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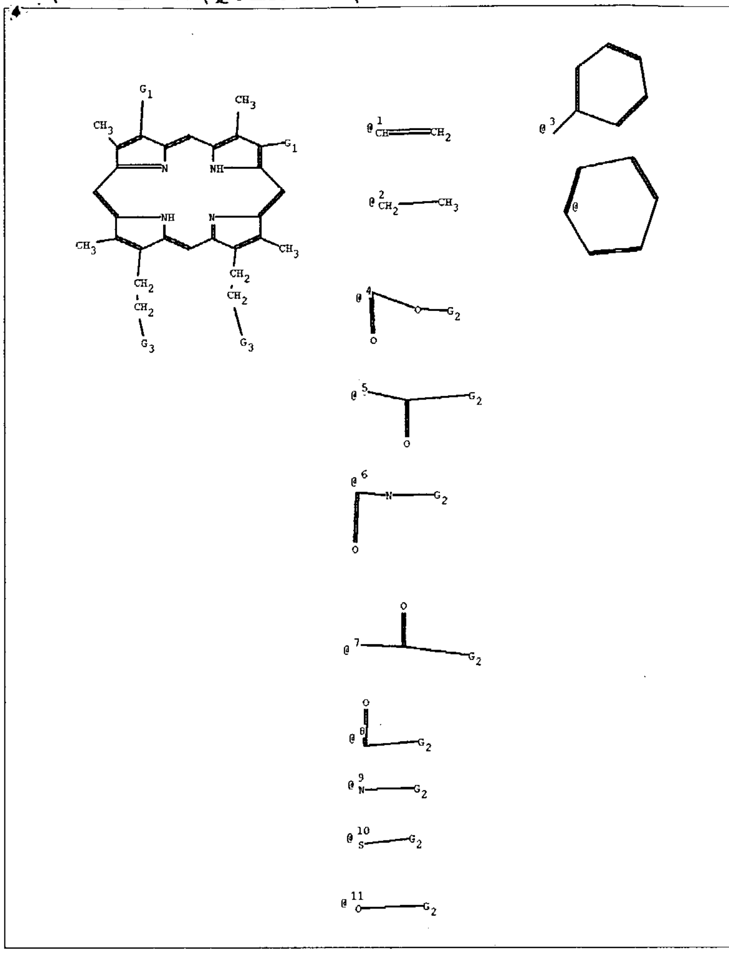

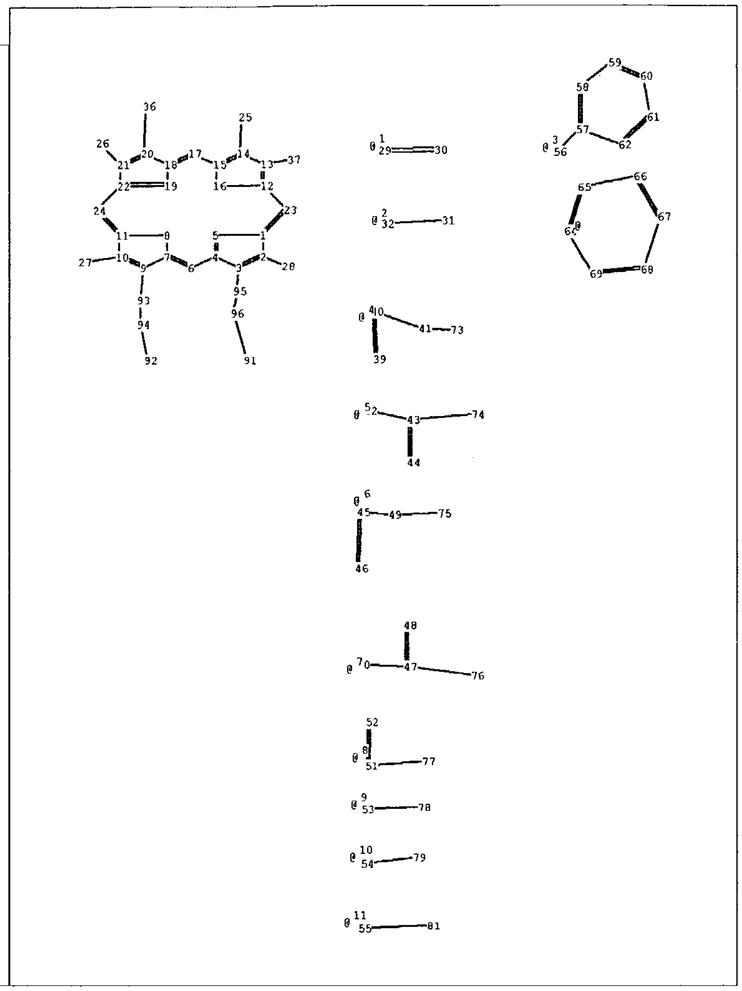

chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 95 96

ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69

chain bonds :
2-28 3-95 9-93 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-96 92-94
93-94 95-96

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
61-62 64-65 64-69 65-66 66-67 67-68 68-69

exact/norm bonds :
7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
53-78 54-79 55-81 91-96 92-94

exact bonds :
2-28 3-95 9-93 10-27 14-25 21-26 29-30 31-32 56-57 93-94
95-96

normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67

67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
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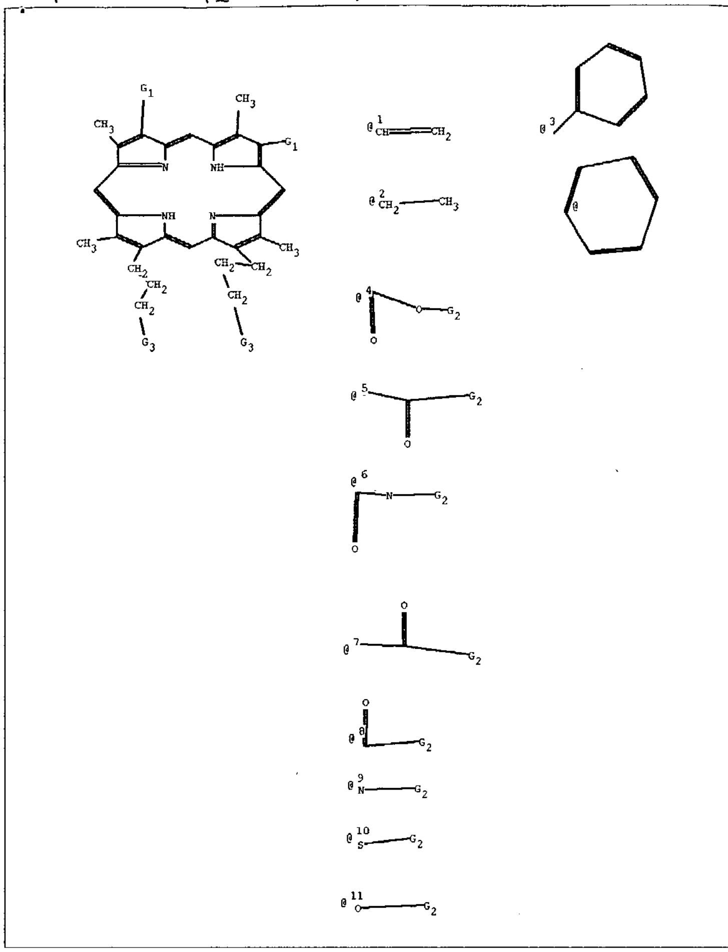
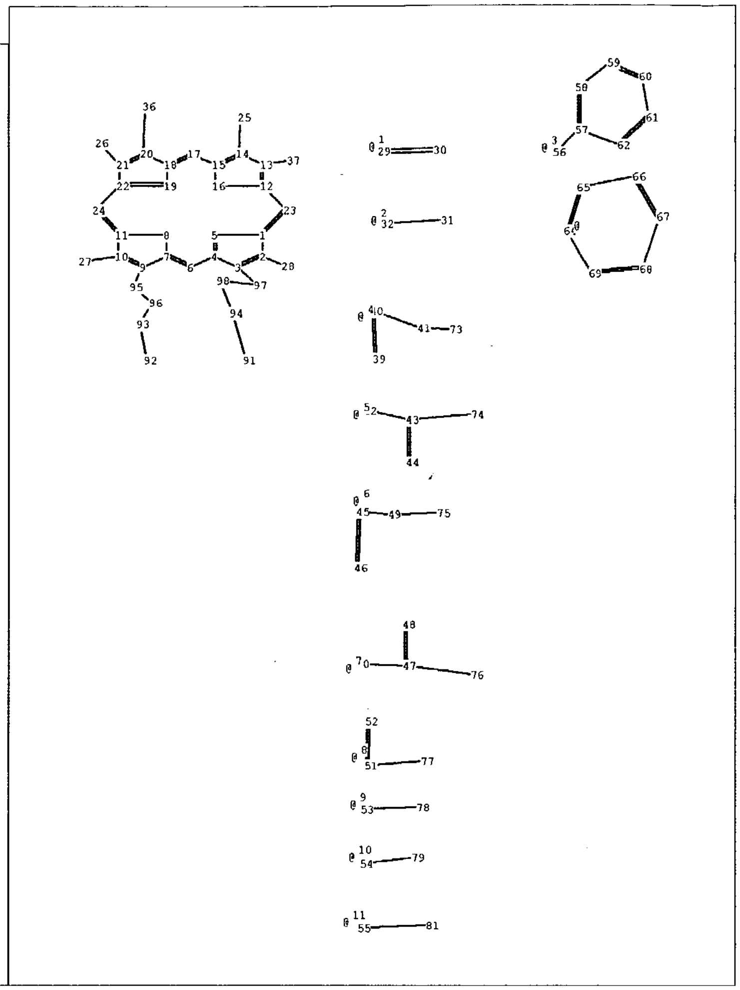
C:\STNEXP4\QUERIES\867b.str





chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 95 96 97 98
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69
chain bonds :
2-28 3-97 9-95 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-96 94-98 95-96 97-98
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
61-62 64-65 64-69 65-66 66-67 67-68 68-69
exact/norm bonds :
7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
53-78 54-79 55-81 91-94 92-93
exact bonds :
2-28 3-97 9-95 10-27 14-25 21-26 29-30 31-32 56-57 93-96
94-98 95-96 97-98
normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67

67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:CLASS 79:CLASS 81:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS
95:CLASS 96:CLASS 97:CLASS 98:CLASS

```
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                  CA/CAplus
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                  changes
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 NEWS 11  MAR 29  No connect hour charges in WPIFV until May 1, 2004
 NEWS 12  MAR 29  New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 13  APR 26  PROMT: New display field available
 NEWS 14  APR 26  IFIPAT/IFIUDB/IFICDB: New super search and display field
                  available
 NEWS 15  APR 26  LITALERT now available on STN
 NEWS 16  APR 27  NLDB: New search and display fields available

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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FILE 'HOME' ENTERED AT 14:24:50 ON 03 MAY 2004
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=> file reg
COST IN U.S. DOLLARS                                      SINCE FILE      TOTAL
                                                               ENTRY    SESSION
FULL ESTIMATED COST                                             7.35       7.35

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STRUCTURE FILE UPDATES:    30 APR 2004  HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES:   30 APR 2004  HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\867a.str

L1       STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1               STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SCREEN SEARCH COMPLETED -    466 TO ITERATE

100.0% PROCESSED     466 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         8025 TO    10615
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> search l1
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
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```
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FULL SCREEN SEARCH COMPLETED -   9800 TO ITERATE

100.0% PROCESSED    9800 ITERATIONS                          13 ANSWERS
SEARCH TIME: 00.00.01

L3           13 SEA SSS FUL L1

=>
Uploading C:\STNEXP4\QUERIES\867b.str

L4      STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l4
SAMPLE SEARCH INITIATED 14:47:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    557 TO ITERATE

100.0% PROCESSED     557 ITERATIONS                           0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        9725 TO    12555
PROJECTED ANSWERS:              0 TO        0

L5            0 SEA SSS SAM L4

=> search l4
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
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FULL SCREEN SEARCH COMPLETED -  11654 TO ITERATE

100.0% PROCESSED   11654 ITERATIONS                           0 ANSWERS
SEARCH TIME: 00.00.01

L6            0 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                    311.68     319.03

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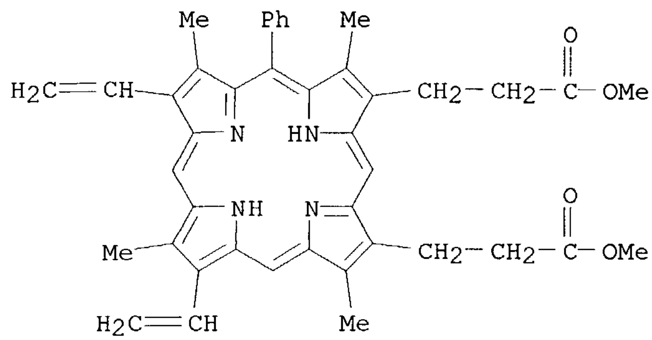
FILE COVERS 1907 - 3 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004 (20040502/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L7 11 L3

=> d fbib ab hitstr 1-11

L7 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:721210 CAPLUS
DN 134:17340
TI Total synthesis and conformational analysis of monophenyl substituted protoporphyrins IX
AU Robinsohn, Adriana E.; Maier, Marta S.; Buldain, Graciela Y.
CS Facultad de Farmacia y Bioquimica, Universidad de Buenos Aires, Buenos Aires, 1113, Argent.
SO Heterocycles (2000), 53(10), 2127-2142
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
OS CASREACT 134:17340
AB The total synthesis of meso-monoaryl protoporphyrins [I; R1 = Ph, R2R3 = H (II)] and [I; R1R3 = H, R2 = Ph (III)] using a MacDonald type [2+2] condensation is described. In this method a bisformyl dipyrrylmethane is treated with a biscarboxydipyrrylmethane. Attempts to obtain the δ-meso-monoaryl protoporphyrin [I; R1R2 = H, R3 = Ph (IV)] by the a,c-biladiene method failed as it could not be prepared starting from its tripyrrene precursor (V). The synthesis of the V is described. Mol. modeling studies allowed us to find the most favorable conformations for II and III. In both porphyrins, the exocyclic Ph group adopts a noncoplanar disposition relative to the plane of the macrocycle. In porphyrin III the macrocycle is nearly planar while nonplanar saddle conformation was obtained for porphyrin II.
IT **309757-24-2P**
RL: PNU (Preparation, unclassified); PREP (Preparation)
(attempted preparation of)
RN 309757-24-2 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethenyl-3,7,12,17-tetramethyl-5-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



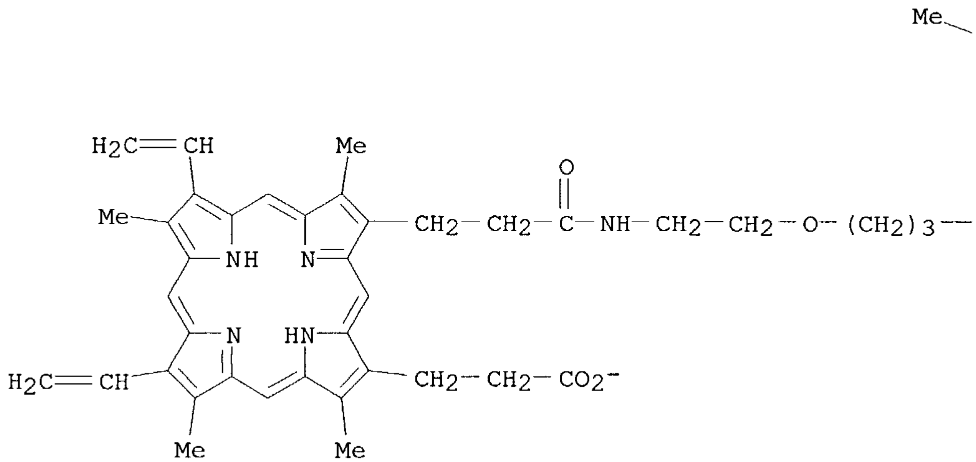
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:367089 CAPLUS
DN 131:110291
TI A convenient synthesis of a Ru(bpy)3-based catenane-type triad and its incorporation into a protein scaffold
AU Hu, Yi-Zhen; Tsukiji, Shinya; Shinkai, Seiji; Hamachi, Itaru
CS Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Fukuoka, 812-8581, Japan
SO Chemistry Letters (1999), (6), 517-518
CODEN: CMLTAG; ISSN: 0366-7022
PB Chemical Society of Japan
DT Journal
LA English
AB A catenated heme cofactor consisting of a sensitizer (Ru(bpy)2L (L = I)), a donor (protoheme) II (R = 4'-methyl-2,2'-bipyridin-4-yl) and an acceptor (cyclobis(paraquat-p-phenylene) (III)) was prepared by stepwise coordination, followed by Fe-insertion. Reconstitution of apomyoglobin with this cofactor afforded a protein-based, noncovalently-linked photosynthetic triad.
IT **231302-74-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of iron porphyrinate ruthenium bipyridine bipryidinocrown ether catenated with cyclobisparaquatphenylene for incorporation in protein scaffold)
RN 231302-74-2 CAPLUS
CN Ruthenium(1+), (2,5,8,11,14,27,30,33,36,39-decaoxa-19,22-diazatetracyclo[38.2.2.116,20.121,25]hexatetraconta-16,18,20(46),21,23,25(45),40,42,43-nonaene-κN19,κN22)[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-[[2-[3-(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')propoxy]ethyl]amino]-3-oxopropyl]-21H,23H-porphine-2-propanoato(1-)](4,4'-dimethyl-2,2'-bipyridine-κN1,κN1')-, (OC-6-43)-, chloride, monohydrochloride, catena compd. with 5,12,19,26-tetraazoniaheptacyclo[24.2.2.22,5.27,10.212,15.216,19.221,24]tetraconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene tetrachloride (1:1) (9CI) (CA INDEX NAME)

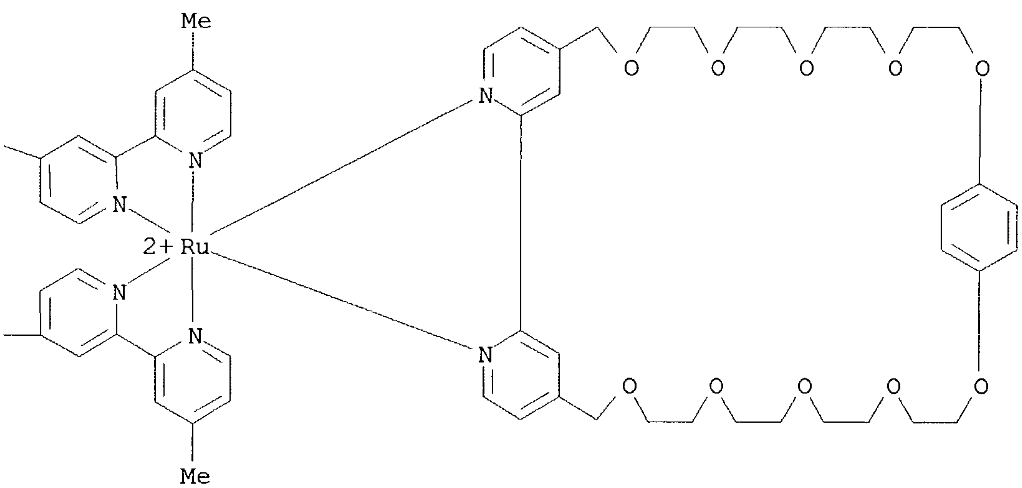
CM 1

CRN 235438-51-4
CMF C96 H110 N11 O14 Ru . Cl H . Cl
CCI CCS

PAGE 1-A



PAGE 1-B



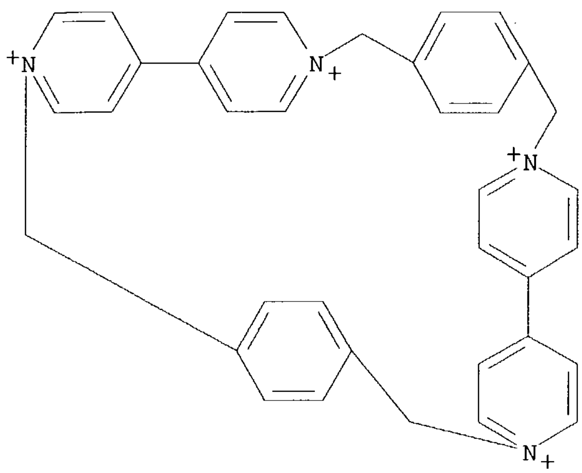
PAGE 2-A

● Cl^-

● HCl

CM 2

CRN 117271-78-0
CMF C36 H32 N4 . 4 Cl



●4 Cl^-

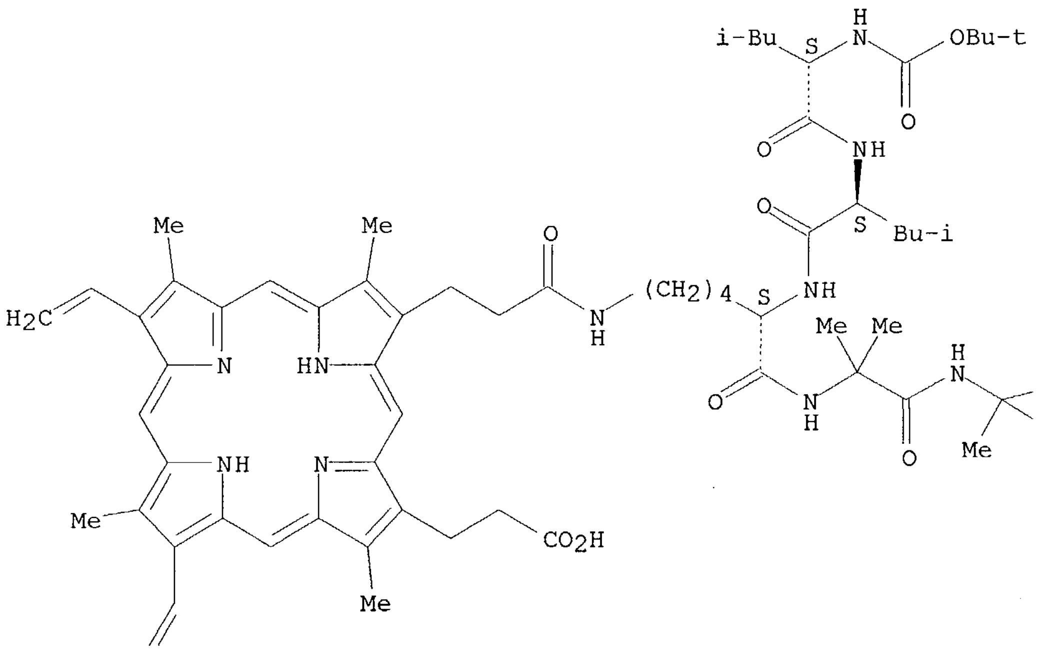
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:528290 CAPLUS
DN 127:109178
TI Molecular Modeling of a Functionalized Aib-Based Octapeptide by Molecular Mechanics Calculations Restrained by NMR and Fluorescence Data in DMSO
AU Pispisa, B.; Palleschi, A.; Amato, M. E.; Segre, A. L.; Venanzi, M.
CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor Vergata, Rome, 00133, Italy
SO Macromolecules (1997), 30(17), 4905-4910
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
AB The structural features of the sequential octapeptide Boc-(Leu)2-Lys(P)-(Aib)2-(Leu)2-Lys(N)-OCMe3, where P is protoporphyrin IX and N is naphthalene, were investigated in DMSO by NMR and fluorescence spectroscopy. Earlier IR, CD, and fluorescence results showed that this compound attains a 310-helical conformation in methanol or water/methanol (75/25, volume/volume). By contrast, the backbone structure in DMSO is destroyed, but the high helix propensity of the Aib residues forces the peptide to attain locally ordered arrangements, reminiscent of β-turn features. Both NMR coupling constant and NOE connectivity data allowed the computation of the structural features of part of the mol., but only their combination with fluorescence results allowed the construction of the whole mol. model. Implications of fluorescence data on the dynamics of internal rotation of the chromophores are briefly discussed.

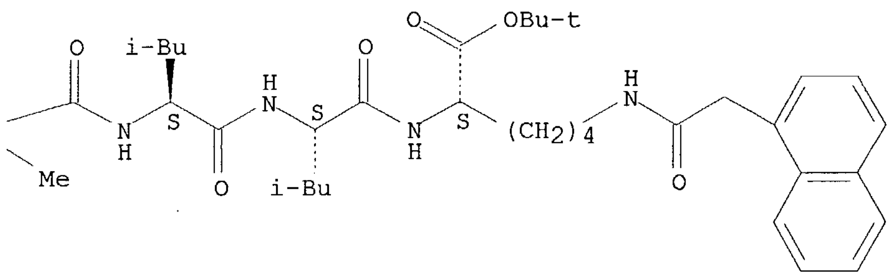
IT **171736-16-6**
RL: PRP (Properties)
(conformation of aminoisobutyric acid peptide by by mol. mechanics calcns. restrained by NMR and fluorescence data in DMSO)
RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

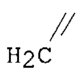
PAGE 1-A



PAGE 1-B

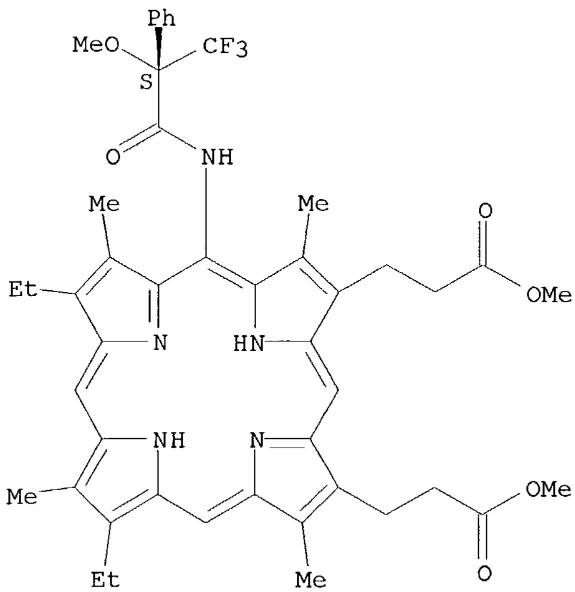


PAGE 2-A



L7 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:641877 CAPLUS
DN 125:328358
TI Synthesis, stereochemical and photophysical studies of chiral mesoporphyrins
AU Poignant, Geraldine; Bourseul, Annie; Geze, Catherine; Plouzennec, Maryvonne Le; Le Maux, Paul; Bondon, Arnaud; Simonneaux, Gerard; Moinet, Claude; Vonarx, Veronique; Patrice, Thierry
CS Lab. Chim. Organometallique Biol., CNRS, Rennes, 35042, Fr.
SO Tetrahedron Letters (1996), 37(42), 7511-7514
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB The synthesis and NMR characterization of chiral mesoporphyrins bearing α-methoxy-α-(trifluoromethyl)phenylacetyl residues are reported. The phototoxicity with circular polarized light and intracellular localization in L1210 cells are also described as preliminary results.
IT **183558-97-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, stereochem. and photophys. studies of chiral mesoporphyrins)
RN 183558-97-6 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-5-[(3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl)amino]-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:189170 CAPLUS
DN 124:317836
TI Conformational Statistics and Energetics Analysis of Sequential Peptides Undergoing Intramolecular Transfer of Excitation Energy
AU Pispisa, B.; Palleschi, A.; Venanzi, M.; Zanotti, G.
CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor Vergata, Rome, 00133, Italy
SO Journal of Physical Chemistry (1996), 100(16), 6835-44
CODEN: JPCHAX; ISSN: 0022-3654
PB American Chemical Society
DT Journal
LA English
AB The photophysics of short linear peptides of general formula Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OCMe3 [AA = Ala, n = 1-4; AA = α-aminoisobutyric acid (Aib), n = 1-2; P = protoporphyrin IX, N = 1-naphthylacetyl] were investigated in 75/25 (volume/volume) water/methanol by steady-state and time-resolved fluorescence expts. Quenching of the excited naphthyl chromophore takes place by electronic energy transfer to the porphyrin ground state, and proceeds on a time scale of 3-8 ns. A minor and slower fluorescence lifetime measures the decay of the exciplexes. Quenching efficiencies exhibit a different trend, depending on whether AA = Ala or Aib, indicating differences in the structural features of the two series of peptides. Consistently, CD spectra suggest that the former compds. populate α-helical structures, while the latter ones possibly attain a 310-helix conformation, in agreement with the proven ability of Aib to form 310-helixes in solution The increased percentage of intramol. H-bonds in the P(Aib)nN as compared to the corresponding P(Ala)nN peptides, as determined by IR spectra in dilute CD3OD or CDCl3 solution, confirms this conclusion. The fluorescence results were satisfactorily described by a dipole-dipole interaction mechanism, provided the mutual orientations of N and P groups are taken into account,

which implies that interconversion among conformational substrates of chromophore linkage is slow on the time scale of the transfer process. Conformational statistics anal. shows a rather wide interprobe separation distance distribution for each peptide, owing to the aliphatic portion of the side-chains carrying the chromophores, but theor. conformational anal. indicates that only a few energetically favored conformers are the major contributors to the energy transfer process.

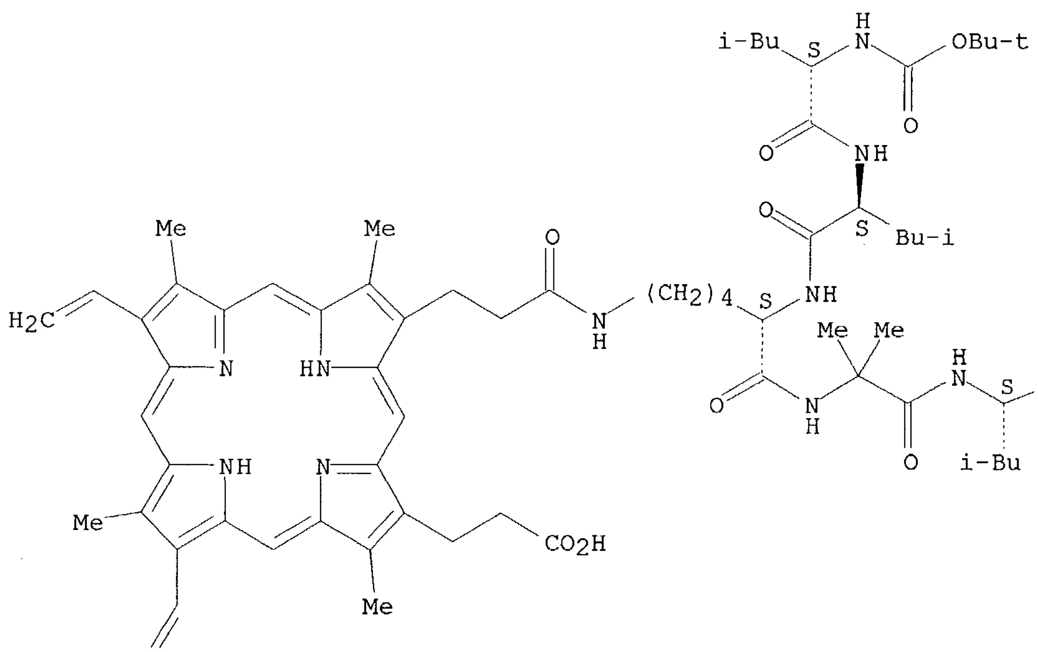
IT **171736-14-4 171736-16-6**
RL: PRP (Properties)
(conformational statistics and energetics anal. of sequential peptides undergoing intramol. transfer of excitation energy)

RN 171736-14-4 CAPLUS

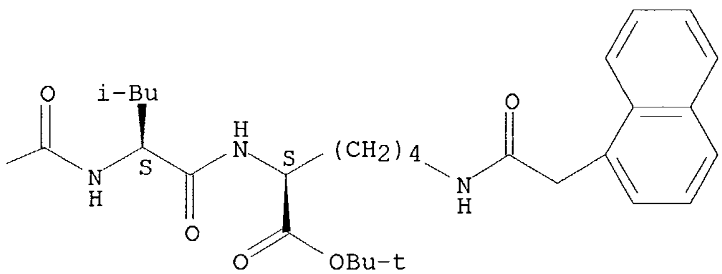
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

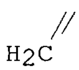
PAGE 1-A



PAGE 1-B



PAGE 2-A

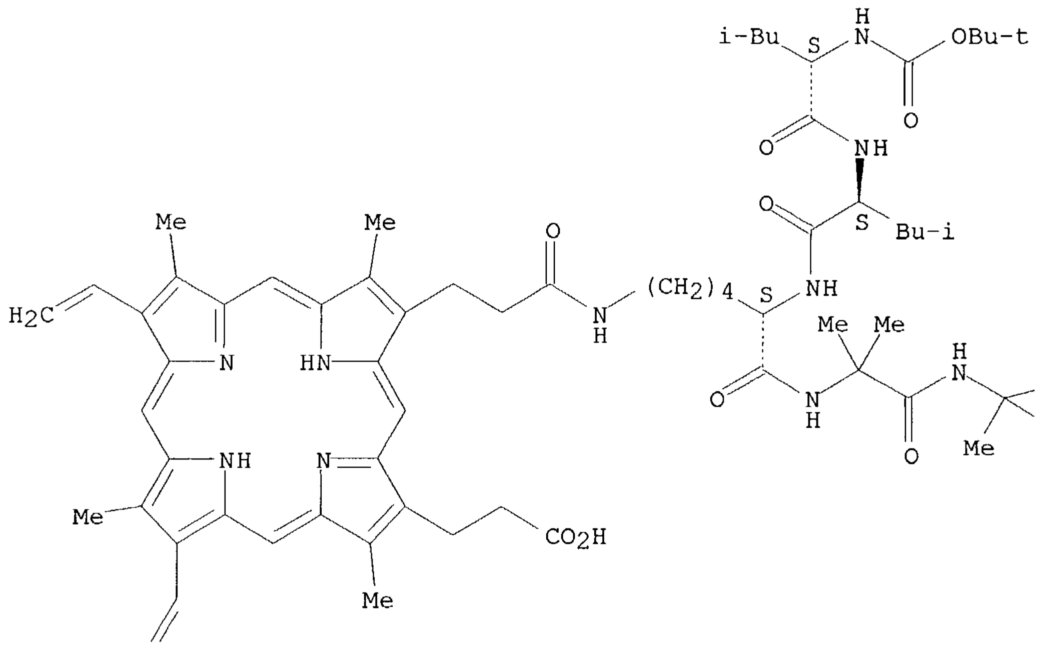


RN 171736-16-6 CAPLUS

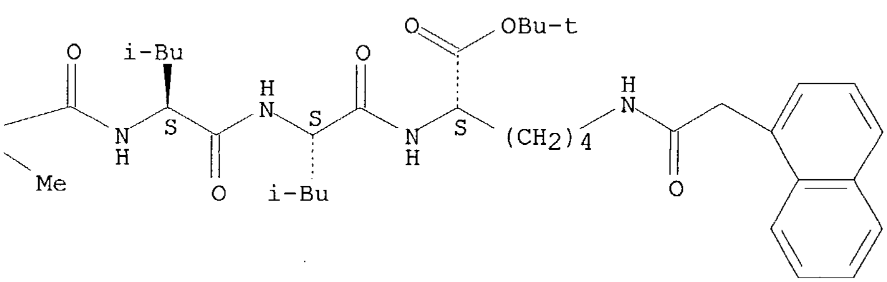
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

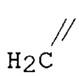
PAGE 1-A



PAGE 1-B



PAGE 2-A

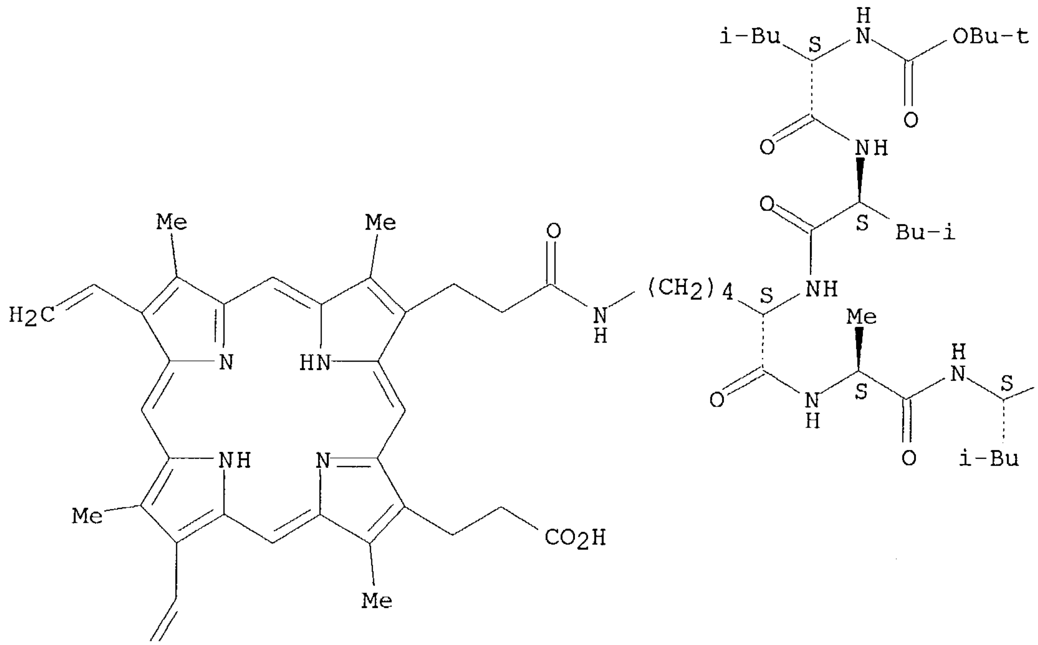


L7 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

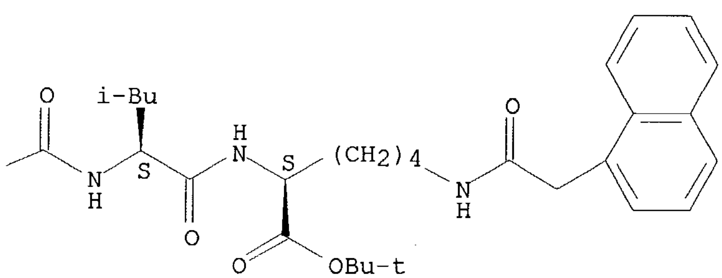
AN 1995:819429 CAPLUS
DN 124:30371
TI Intramolecular electronic energy transfer in peptides carrying naphthalene and protoporphyrin molecules: a spectroscopy and conformational statistics investigation
AU Pispisa, B.; Venanzi, M.; Palleschi, A.; Zanotti, G.
CS Dip. Science, Univ. Rome, Rome, 00133, Italy
SO Biopolymers (1995), 36(4), 497-510
CODEN: BIPMAA; ISSN: 0006-3525
PB Wiley
DT Journal
LA English
AB Short linear peptides, carrying an AA spacer in the backbone chain (AA = Aib or Ala) and naphthalene (N) and protoporphyrin IX (P) covalently bound to ε-amino groups of lysine side chains, were synthesized. The general formula is Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OtBu (n = 0-2). The photophys. behavior of these compds. was investigated in water/methanol (75/25, volume/volume) solution by steady-state and time-resolved fluorescence expts. Quenching of excited naphthyl chromophore takes place by electronic energy transfer to the porphyrin ground state and proceeds on a time scale of 3-8 ns, while a minor and slower (≈45 ns) fluorescence lifetime measures the decay of the exciplexes. The results were compared with those obtained earlier for the P(Ala)nN peptides (n = 0-4) in methanol solution, showing that addition of water does not significantly alter the dynamic relaxation behavior of the systems investigated, but affects the dissipation mechanism of the energy transferred to P. Quenching efficiencies from both fluorescence intensity and fluorescence lifetime measurement follow a different trend as the number of AA units increases, depending on whether AA = Aib or Ala, indicating that there are differences in the structural features of the two series of peptides. Consistently, CD spectral results suggest that the former compds. attain ordered conformations, possibly of the 310-helical type, while the latter populate α-helical structures to an extent depending on the chain length. Their IR data in dilute CD3OD or CDCl3 solution confirm this conclusion in that there is an increased percentage of intramol. H bonds in the P(Aib)nN as compared to the corresponding P(Ala)nN peptides. The photophys. results can be well described by a long-range dipole-dipole interaction model, provided the separation distances distribution and mutual orientation of N and P groups are taken into account. The need for using the angular relationships between the probes implies that interconversion among conformational substrates of chromophore linkages is slow on the time scale of the transfer process, very likely because of both the amide bond in the linkages and the bulkiness of the donor-acceptor pair.
IT **171736-17-7 171736-18-8 171736-19-9**
RL: PRP (Properties)
(intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)
RN 171736-17-7 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

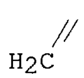
PAGE 1-A



PAGE 1-B



PAGE 2-A

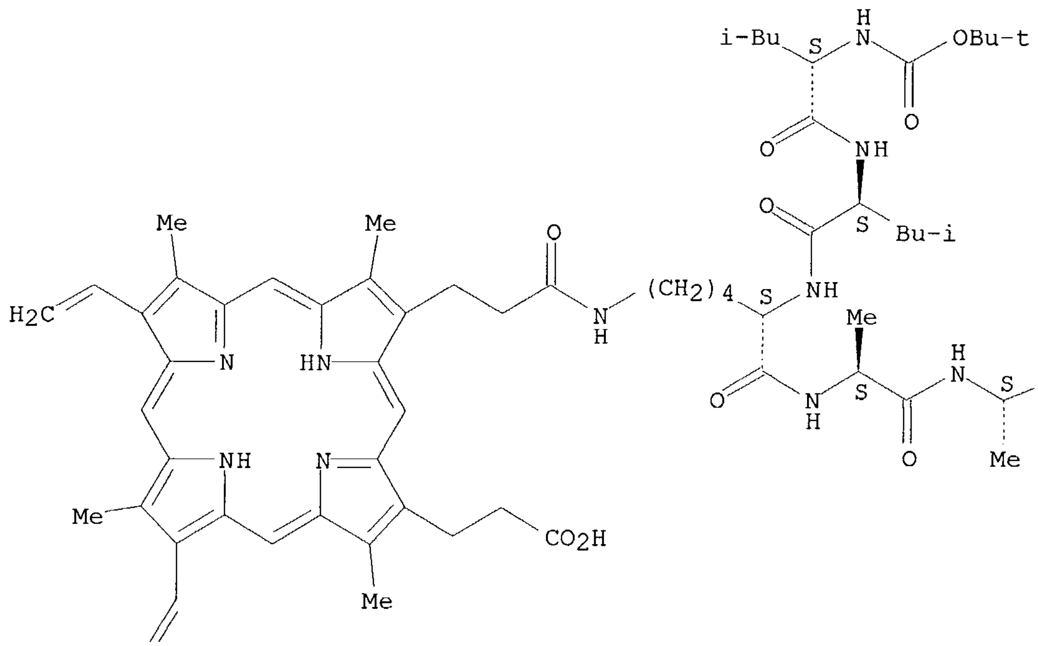


RN 171736-18-8 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-

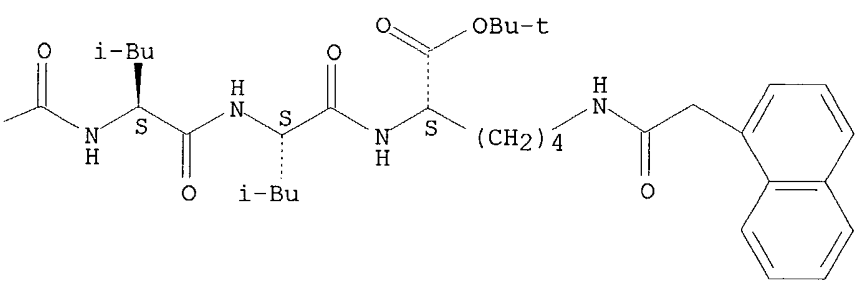
dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-alanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

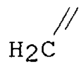
PAGE 1-A



PAGE 1-B



PAGE 2-A

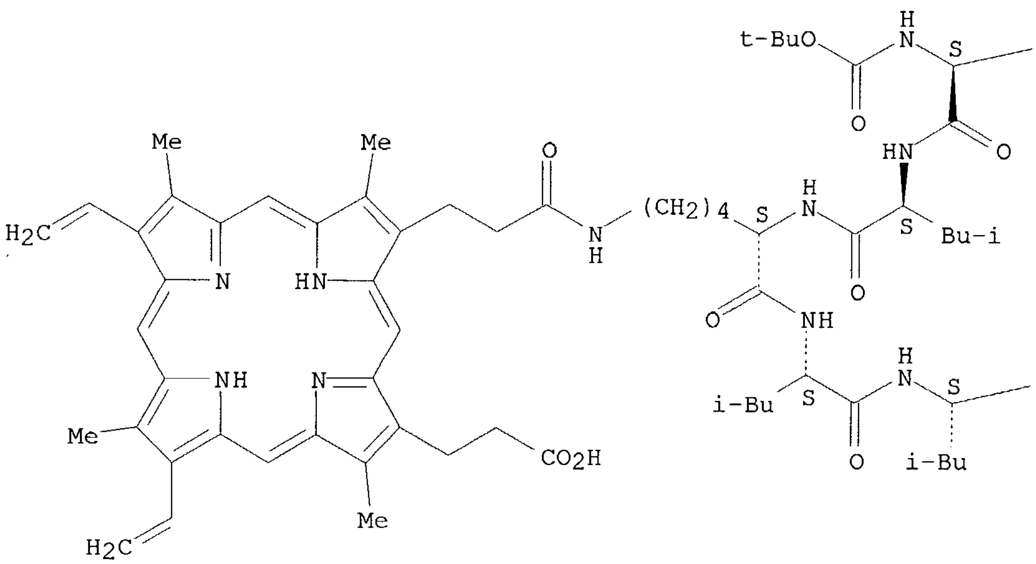


RN 171736-19-9 CAPLUS

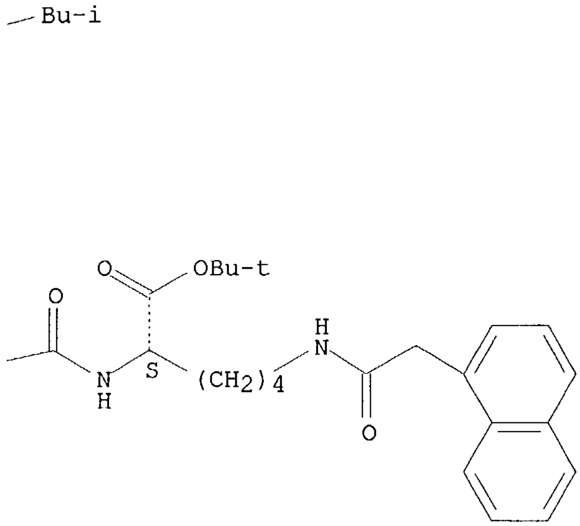
CN L-Lysine, N2-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



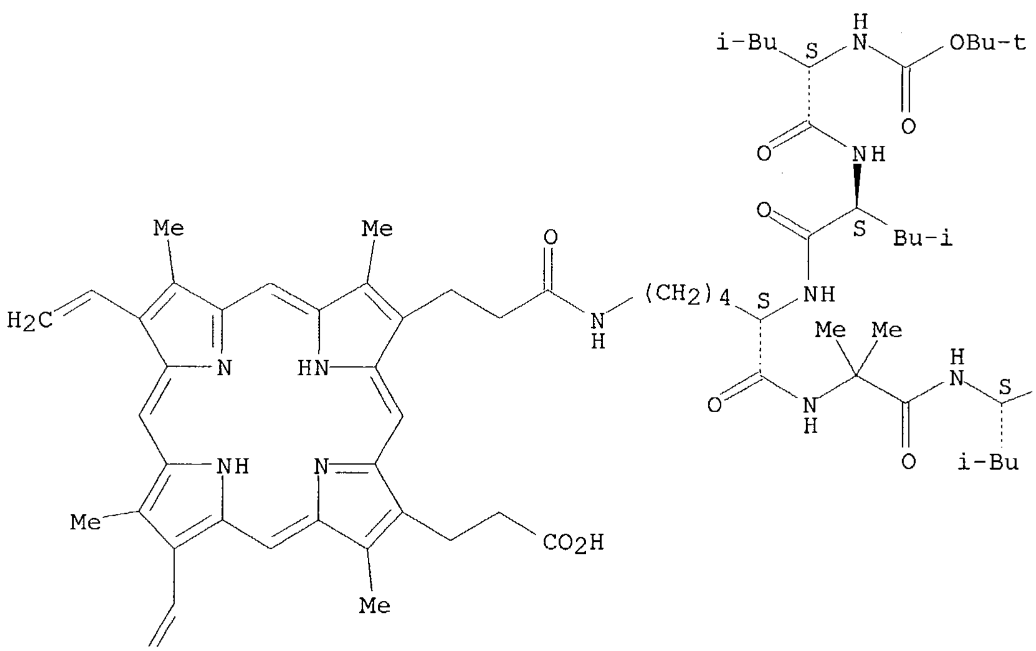
IT **171736-14-4P 171736-16-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)

RN 171736-14-4 CAPLUS

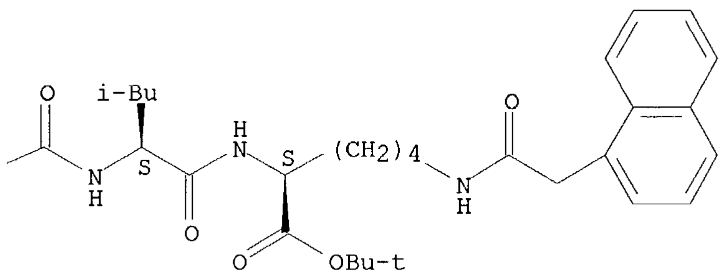
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

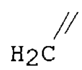
PAGE 1-A



PAGE 1-B



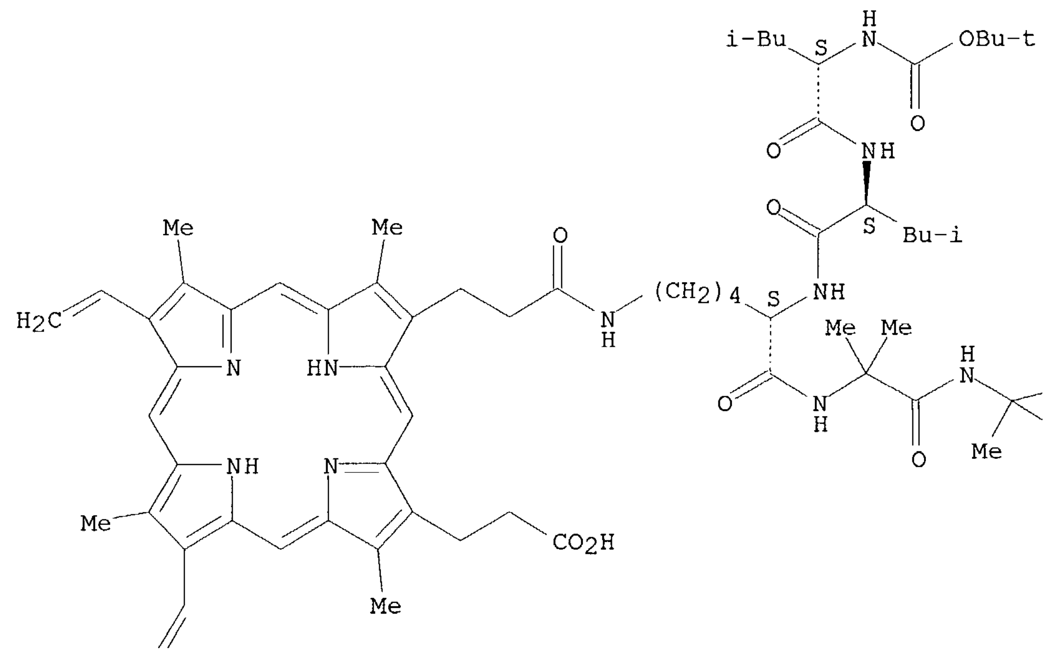
PAGE 2-A



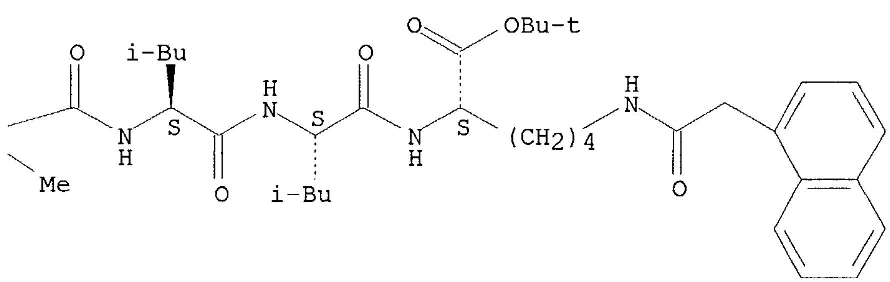
RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

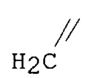
PAGE 1-A



PAGE 1-B

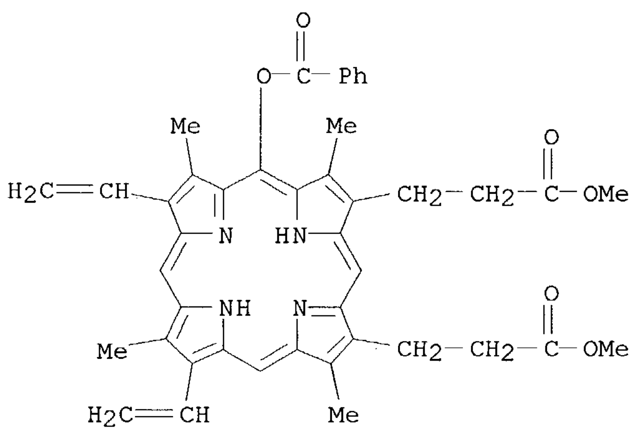


PAGE 2-A



L7 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:21587 CAPLUS
DN 108:21587
TI Synthetic and biosynthetic studies of porphyrins. Part 11. The synthesis of meso oxygenated protoporphyrins
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (2), 307-12
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 108:21587
AB Protoporphyrin IX di-Me ester (I; R-R3 = H) was treated with (BzO)2 to give a mixture of 4 meso-benzoyloxy derivs. I (R = OBz, R1-R3 = H; R1 = OBz, R = R2 = R3 = H; R2 = OBz, R = R1 = R3 = H; R3 = OBz, R-R2 = H) (II). The mixture II was hydrolyzed to the corresponding oxyporphyrins, complexed with Fe, and oxidized with mol. O to give 4 biliverdin di-Me esters III. Conditions for the HPLC sepns. of II and III are discussed.
IT **83807-58-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and basic hydrolysis of)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



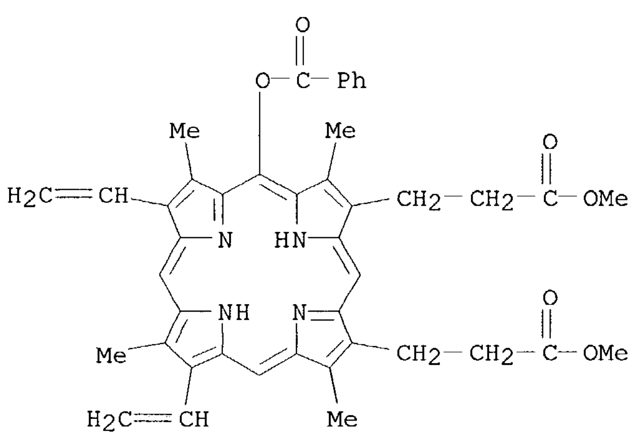
L7 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:202979 CAPLUS
DN 104:202979
TI On the mechanism of the chemical and enzymic oxygenations of α-oxyprotohemin IX to iron·biliverdin IXα
AU Sano, Seiyo; Sano, Toyo; Morishima, Isao; Shiro, Yoshitugu; Maeda, Yutaka
CS Dep. Public Health, Fac. Med., Kyoto, 606, Japan
SO Proceedings of the National Academy of Sciences of the United States of America (1986), 83(3), 531-5
CODEN: PNASA6; ISSN: 0027-8424
DT Journal
LA English
AB α-Oxyprotohemin IX (I), an early intermediate in heme catabolism, was synthesized and its autoxidn. to biliverdin IXα was studied. In

anaerobic aqueous pyridine, I (hexacoordinated) underwent autoredn. to yield an Fe(II)-I π-neutral radical bis(pyridine) complex, which reacted with an equimolar amount of O2 to give verdohemochrome IXα (II)-pyridine and CO in 75-80% yield via an intermediate with an absorption maximum at 893 nm. II did not react with further O2. Reconstituted apomyoglobin-I complex (pentacoordinated) reacted with an equimolar amount of O2 to form an Fe(II)-oxyporphyrin π-neutral radical intermediate, which rearranged to a green compound (λmax 660 and 704 nm) with elision of CO. The green product, which is probably an apomyoglobin-verdoheme π-radical complex, reacted with another equimolar amount of O2 to give Fe(III)-biliverdin IXα. Demetallation of this gave biliverdin IXα in an overall yield of 70-75%. Apparently, the 2-step sequence of oxyheme autoxidn. in the presence of apomyoglobin is α-oxyprotoheme IX → II π-radical → Fe(III)-biliverdin IXα (with CO leaving in the 1st step). A similar mechanism may prevail in vivo.the hexa- and pentacoordinated Fe(II) π-radical form of the oxyporphyrin is crucial in triggering the autoxidn. of the complex to verdohemochrome IXα. The hexa- and pentacoordinated Fe(II) π-radical form of the oxyporphyrin was crucial in triggering the autoxidn. of the complex to II. Further oxygenation of II to Fe(III)-biliverdin IXα occurred only in the pentacoordinated apomyoglobin-verdoheme Fe(II) complex.

IT **83807-58-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and deprotection of and iron insertion in)

RN 83807-58-3 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:45748 CAPLUS

DN 98:45748

TI Heminopeptide complexes which are models of an "active center" of oxygen-transferring hemoproteides. Synthesis and properties

AU Kazakova, N. A.; Radyukhin, V. A.; Luzgina, V. N.; Filippovich, E. I.; Kamyshan, N. V.; Kudryavtseva, E. V.; Evstigneeva, R. P.

CS Mosk. Inst. Tonkoi Khim. Tekhnol., Moscow, USSR

SO Zhurnal Obshchei Khimii (1982), 52(8), 1896-906
CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

AB Unsym. 6(7), 7(6)-bis(amino acyl)peptide derivs. of protohemin IX (models of active centers of Hb and myoglobin) were prepared The stability consts. were determined for the mono- and bis(amino acyl)peptide derivs. of protohemin IX with axial N-containing ligands (1-methylimidazole); the covalently-bound peptide has a stabilizing effect on the formation and stability of the 5-coordinate complexes. The hydrophobic spatial environment around the Fe ion of the ferroporphyrin 5-coordinate complexes affects their stability toward oxidation and their ability to coordinate CO at room temperature

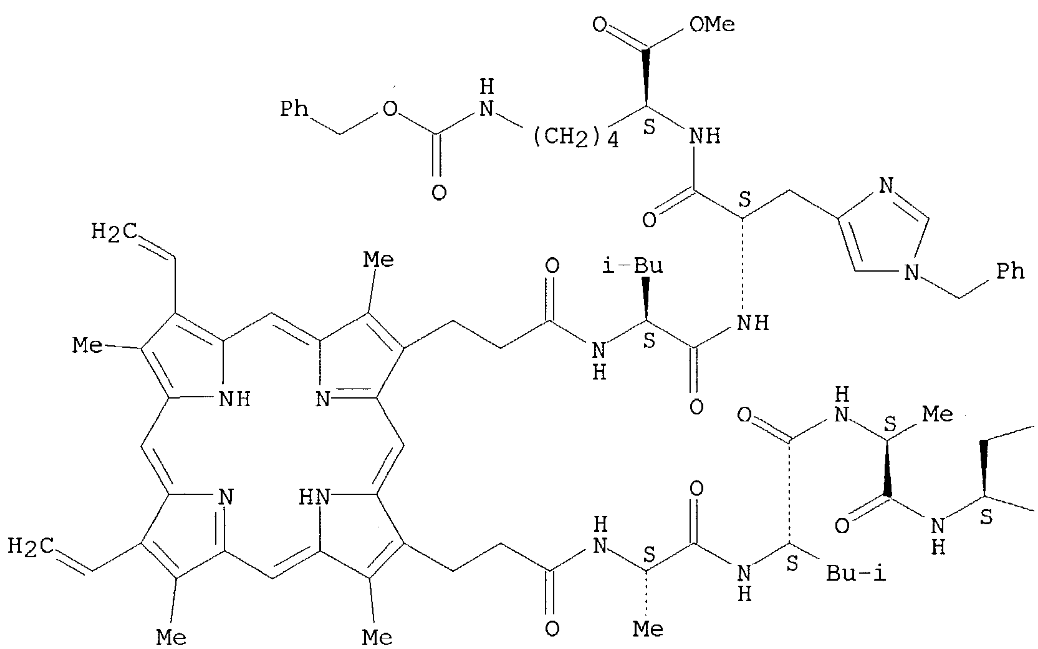
IT **83841-59-2D,** iron complexes with methylimidazole and pyridine
RL: PRP (Properties)
(stability consts. of)

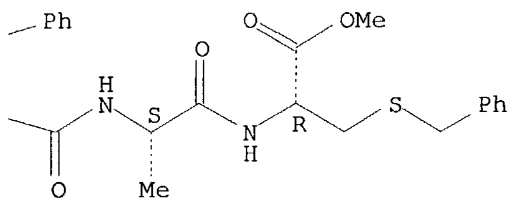
RN 83841-59-2 CAPLUS

CN L-Cysteine, N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl-L-leucyl-L-alanyl-L-phenylalanyl-L-alanyl-S-(phenylmethyl)-, 6-methyl ester, (1→1')-amide with L-leucyl-1-(phenylmethyl)-L-histidyl-N6-[(phenylmethoxy)carbonyl]-L-lysine methyl ester (9CI) (CA INDEX NAME)

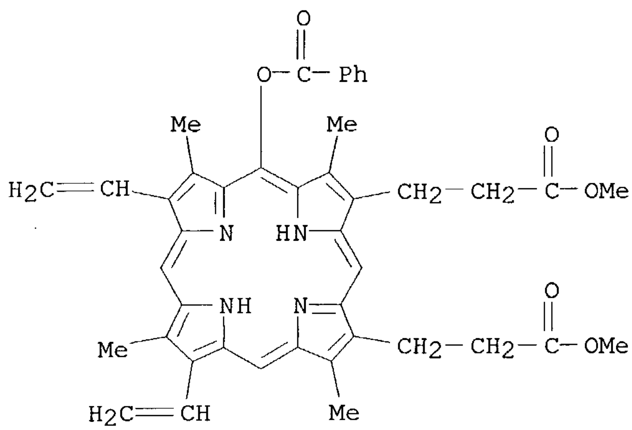
Absolute stereochemistry.

PAGE 1-A





L7 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:615860 CAPLUS
DN 97:215860
TI Synthesis of the four meso-oxyprotoporphyrin isomers
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Chemical Communications (1982), (14), 794-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB Oxidation of protoporphyrin IX di-Me ester with Bz_2O_2 in PhCl at 95° for 5 min gave a mixture of the 4 title compds. I (1 of R-R3 = OBz, other R groups = H) in 20% yield. I were separated by h.p.l.c. and identified by conversion to the corresponding biliverdins by passage in a 1:1 $CHCl_3/C_6H_6$ solution through a column of basic Al_2O_3, conversion to Fe complexes, and oxygenation in pyridine.
IT **83807-58-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to corresponding biliverdin)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:621062 CAPLUS
DN 93:221062
TI Unsymmetrical 6,7-peptidylprotohemin IX
IN Molokoedov, A. S.; Radyukhin, V. A.; Filippovich, E. I.; Evstigneeva, R. P.
PA Moscow Institute of Fine Chemical Technology, USSR
SO U.S.S.R.
From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1980, (7), 117.
CODEN: URXXAF
DT Patent
LA Russian
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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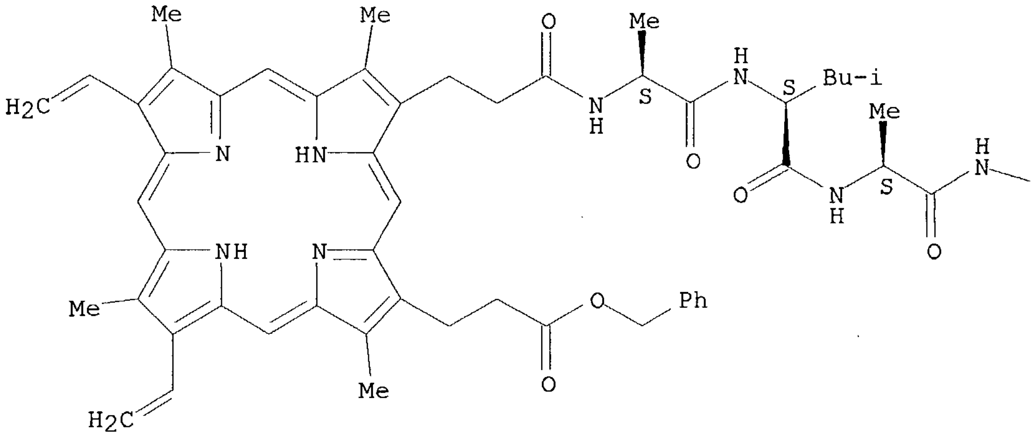
PI	SU 717039	T	19800225	SU 1978-2606603	19780331
				SU 1978-2606603	19780331

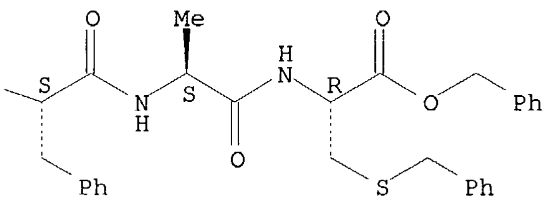
AB Title compds. I [R = PhCH2O, Leu-His(CH2Ph)-Lys(Z)-OMe (Z = PhCH2O2C), R1 = Leu-His-Ala-Lys(Z)-Gly-Cys(CH2Ph)-OCH2Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH2Ph)-OCH2Ph; R = Leu-His-Ala-Lys(Z)-Gly-Cys(CH2Ph)-OCH2Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH2Ph)-OCH2Ph, R1 = PhCH2O, Leu-His(CH2Ph)-Lys(Z)-OMe] were prepared by esterifying I (R = PhCH2O, R1 = HO; R = HO, R1 = PhCH2O) with C6H5OH by the mixed anhydride method with ClCO2Et and condensing the resulting pentachlorophenyl active esters with the appropriate hexapeptides in 2.5-3 M urea solution at 40-45°.
IT **75561-35-2DP,** complex with iron chloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 75561-35-2 CAPLUS
CN L-Cysteine, N-[N-[N-[N-[N-[N-[3-[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-oxo-3-(phenylmethoxy)propyl]-21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl]-L-leucyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]-S-(phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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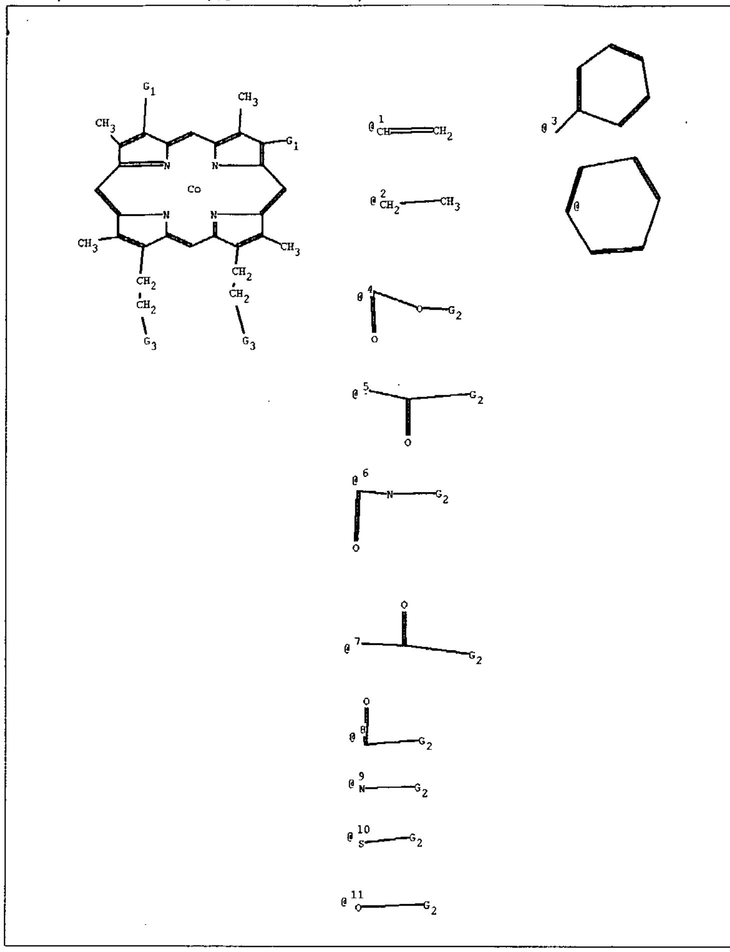

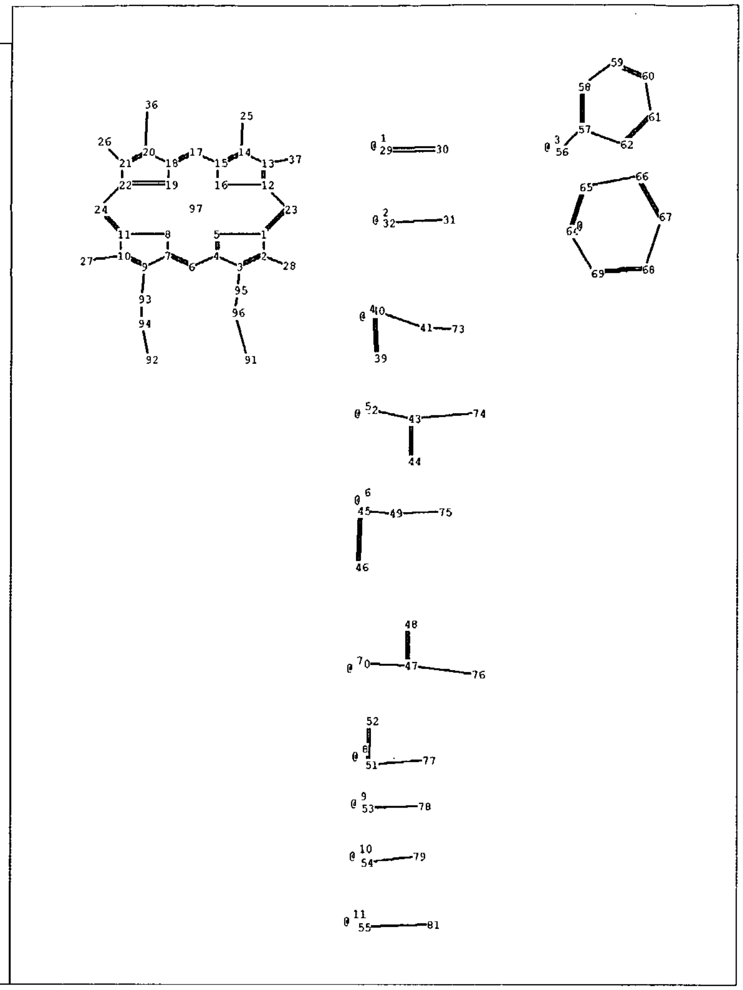

chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 95 96 97
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69
chain bonds :
2-28 3-95 9-93 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-96 92-94
93-94 95-96
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
61-62 64-65 64-69 65-66 66-67 67-68 68-69
exact/norm bonds :
7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
53-78 54-79 55-81 91-96 92-94
exact bonds :
2-28 3-95 9-93 10-27 14-25 21-26 29-30 31-32 56-57 93-94
95-96
normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67

67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
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95:CLASS 96:CLASS 97:CLASS

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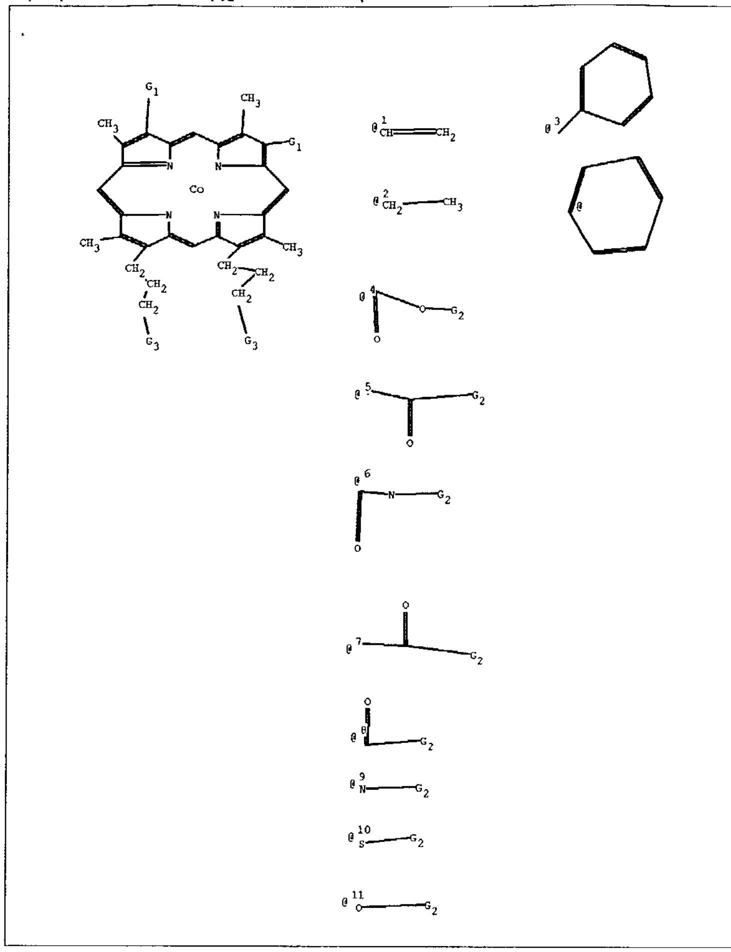

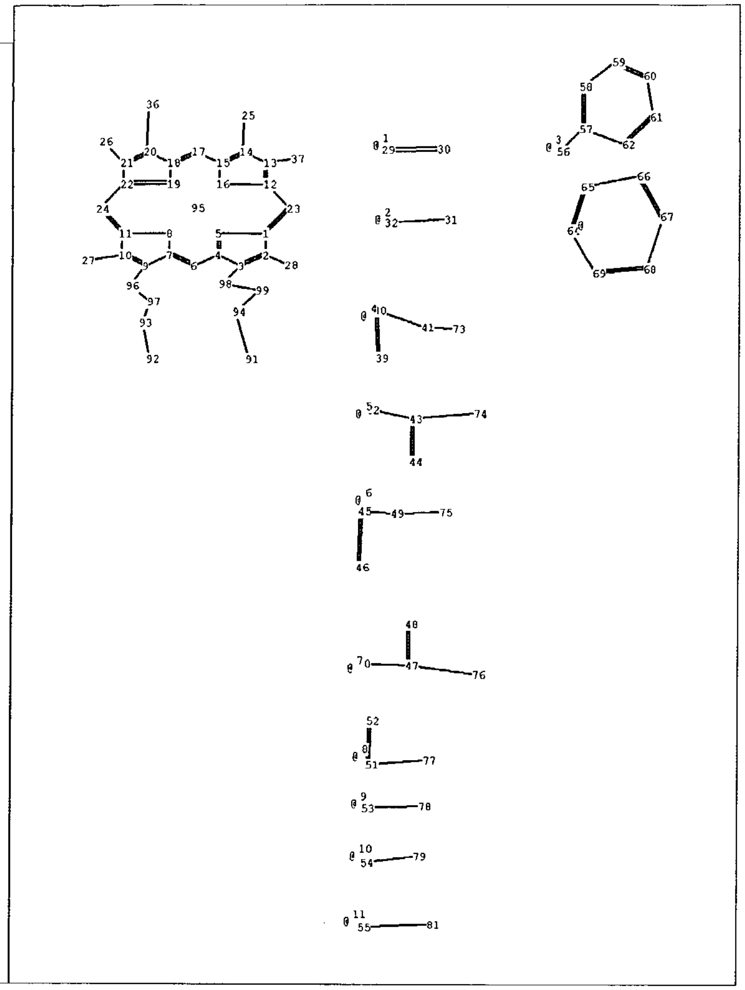

chain nodes :
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47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 95 96 97 98 99
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69
chain bonds :
2-28 3-98 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-97 94-99 96-97 98-99
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
61-62 64-65 64-69 65-66 66-67 67-68 68-69
exact/norm bonds :
7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
53-78 54-79 55-81 91-94 92-93
exact bonds :
2-28 3-98 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-97
94-99 96-97 98-99
normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67

67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
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95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS

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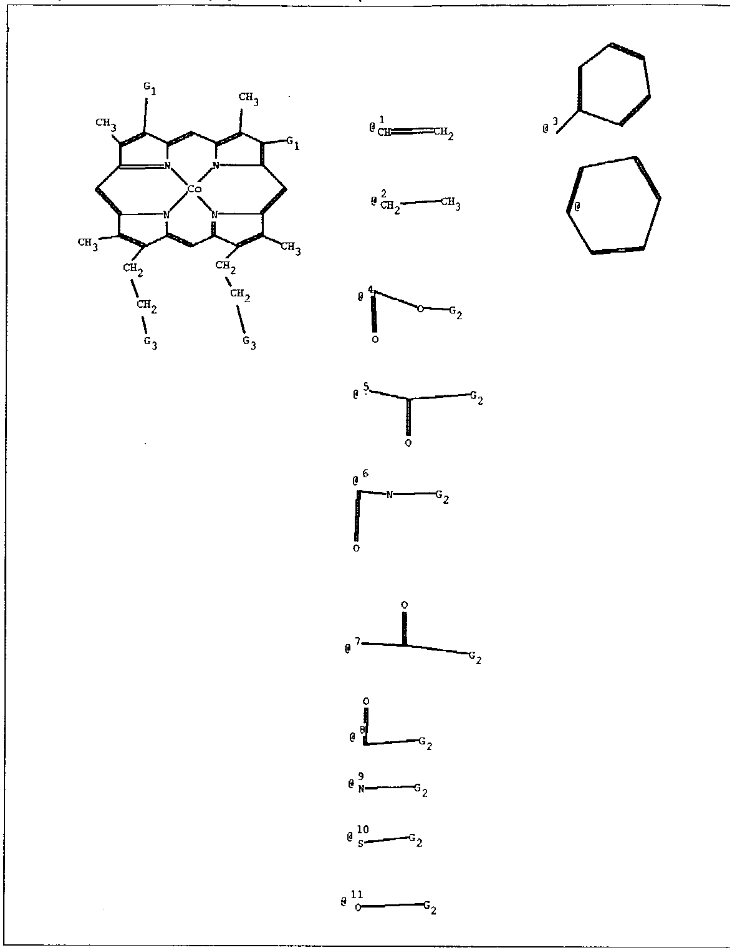

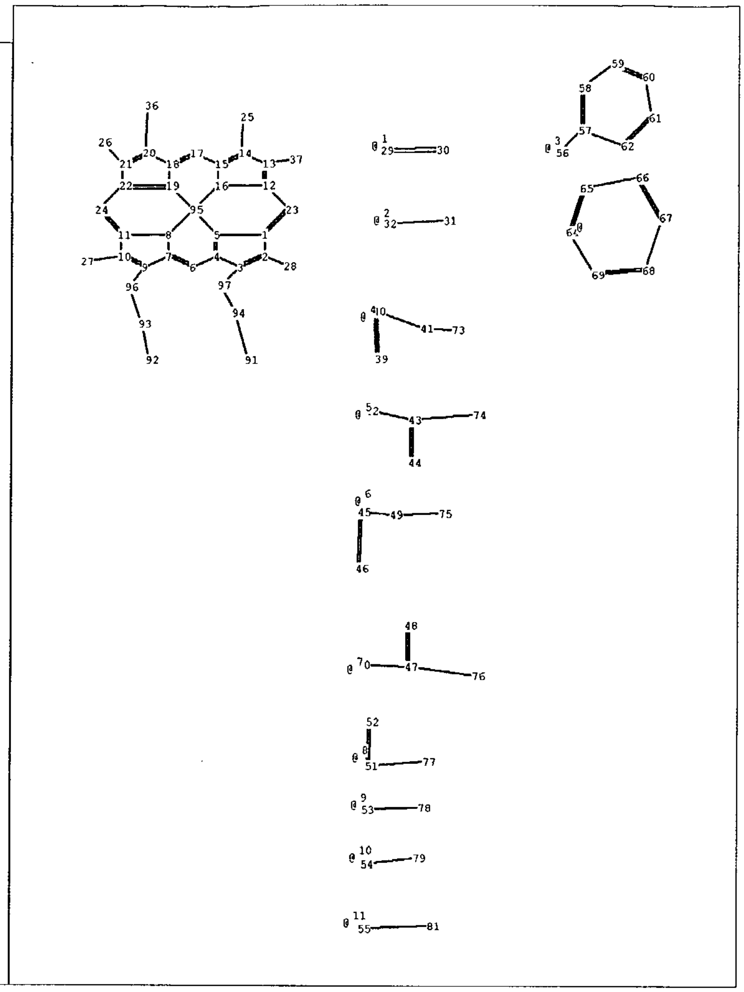

chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 96 97
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 95
chain bonds :
2-28 3-97 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-96 94-97
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-95 6-7 7-8 7-9 8-11 8-95
9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
16-95 17-18 18-19 18-20 19-22 19-95 20-21 21-22 22-24 57-58
57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
68-69
exact/norm bonds :
5-95 7-8 8-11 8-95 12-16 13-37 15-16 16-95 19-95 20-36 39-40
40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
49-75 51-52 51-77 53-78 54-79 55-81 91-94 92-93
exact bonds :
2-28 3-97 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-96
94-97
normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24

57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
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10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
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45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
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59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
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95:CLASS 96:CLASS 97:CLASS

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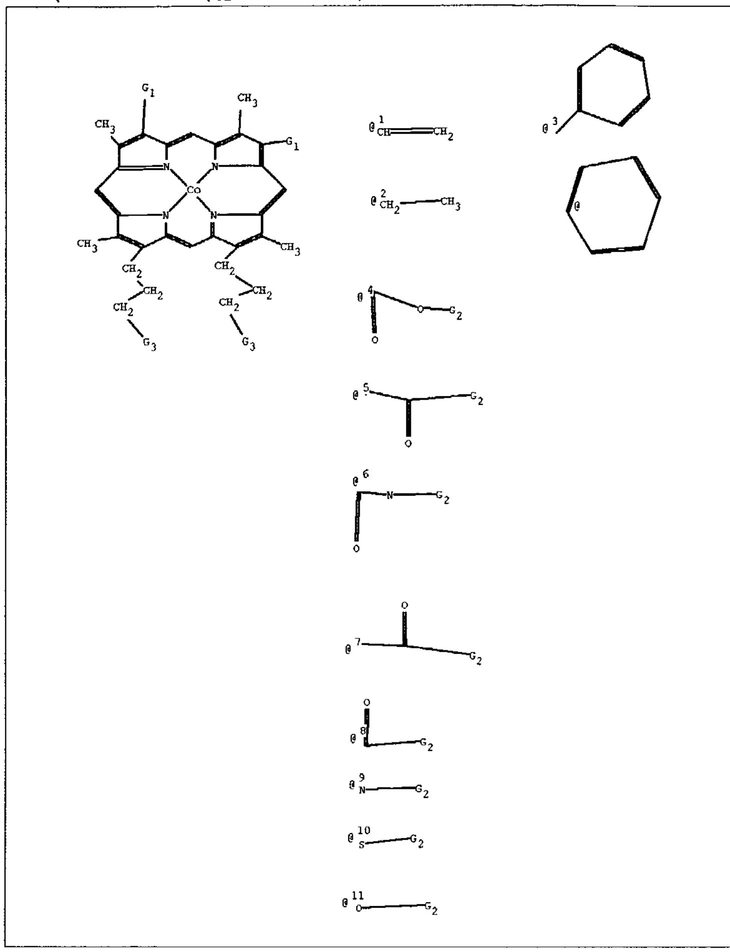

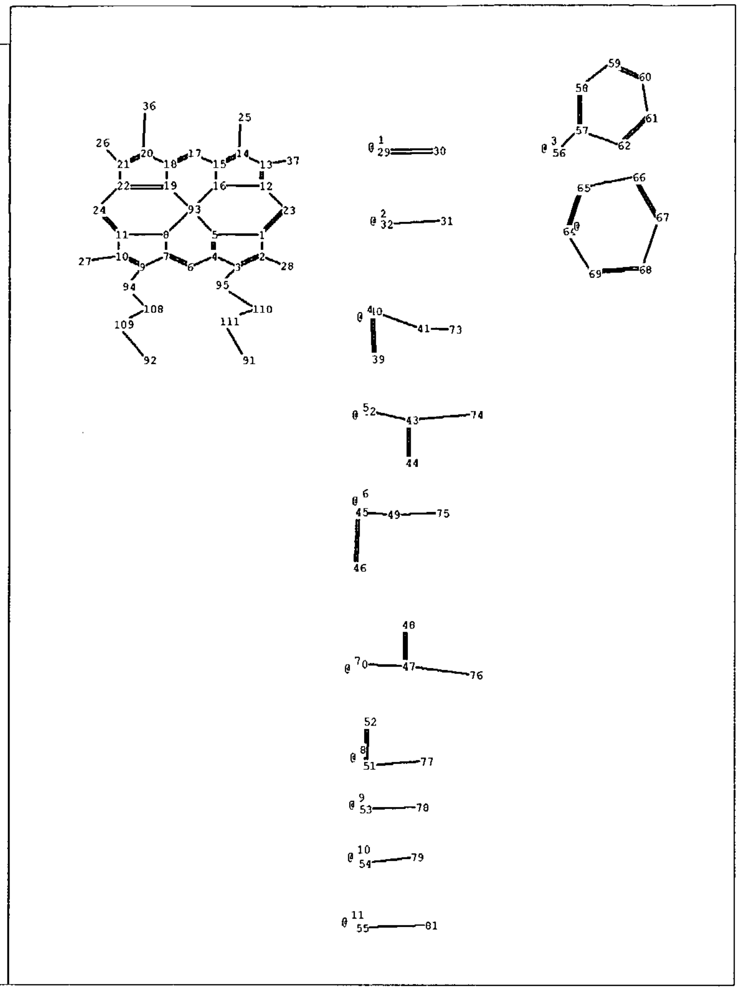

chain nodes :
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47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 94 95 108 109 110 111
ring nodes :
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21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 93
chain bonds :
2-28 3-95 9-94 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-111 92-109
94-108 95-110 108-109 110-111
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-93 6-7 7-8 7-9 8-11 8-93
9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
16-93 17-18 18-19 18-20 19-22 19-93 20-21 21-22 22-24 57-58
57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
68-69
exact/norm bonds :
5-93 7-8 8-11 8-93 12-16 13-37 15-16 16-93 19-93 20-36 39-40
40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
49-75 51-52 51-77 53-78 54-79 55-81 91-111 92-109
exact bonds :
2-28 3-95 9-94 10-27 14-25 21-26 29-30 31-32 56-57 94-108
95-110 108-109 110-111
normalized bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24

57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
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45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
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68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
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95:CLASS 108:CLASS 109:CLASS 110:CLASS 111:CLASS

```
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PASSWORD:
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 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  JAN 27  Source of Registration (SR) information in REGISTRY updated
                  and searchable
 NEWS  4  JAN 27  A new search aid, the Company Name Thesaurus, available in
                  CA/CAplus
 NEWS  5  FEB 05  German (DE) application and patent publication number format
                  changes
 NEWS  6  MAR 03  MEDLINE and LMEDLINE reloaded
 NEWS  7  MAR 03  MEDLINE file segment of TOXCENTER reloaded
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 NEWS 10  MAR 29  WPIFV now available on STN
 NEWS 11  MAR 29  No connect hour charges in WPIFV until May 1, 2004
 NEWS 12  MAR 29  New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 13  APR 26  PROMT: New display field available
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 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
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FILE 'HOME' ENTERED AT 14:24:50 ON 03 MAY 2004

=>
=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
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                                                 ENTRY    SESSION
FULL ESTIMATED COST                               7.35       7.35

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STRUCTURE FILE UPDATES:    30 APR 2004  HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES:   30 APR 2004  HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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http://www.cas.org/ONLINE/DBSS/registryss.html

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L1       STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 14:46:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     466 TO ITERATE

100.0% PROCESSED     466 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:         8025 TO    10615
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> search l1
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:46:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    9800 TO ITERATE

100.0% PROCESSED    9800 ITERATIONS                             13 ANSWERS
SEARCH TIME: 00.00.01

L3           13 SEA SSS FUL L1
```

```
=>
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L4      STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4                STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SEARCH INITIATED 14:47:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    557 TO ITERATE

100.0% PROCESSED     557 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         9725 TO    12555
PROJECTED ANSWERS:               0 TO        0

L5             0 SEA SSS SAM L4

=> search l4
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:47:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  11654 TO ITERATE

100.0% PROCESSED   11654 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS                                  SINCE FILE     TOTAL
                                                           ENTRY   SESSION
FULL ESTIMATED COST                                       311.68    319.03

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FILE COVERS 1907 - 3 May 2004  VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004  (20040502/ED)
```

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> s l3
L7          11 L3

=> d fbib ab hitstr 1-11

L7   ANSWER 1 OF 11  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2000:721210  CAPLUS
DN   134:17340
TI   Total synthesis and conformational analysis of monophenyl substituted
     protoporphyrins IX
AU   Robinsohn, Adriana E.; Maier, Marta S.; Buldain, Graciela Y.
CS   Facultad de Farmacia y Bioquimica, Universidad de Buenos Aires, Buenos
     Aires, 1113, Argent.
SO   Heterocycles (2000), 53(10), 2127-2142
     CODEN: HTCYAM; ISSN: 0385-5414
PB   Japan Institute of Heterocyclic Chemistry
DT   Journal
LA   English
OS   CASREACT 134:17340
AB   The total synthesis of meso-monoaryl protoporphyrins [I; R1 = Ph, R2R3 =
     (II)] and [I; R1R3 = H, R2 = Ph (III)] using a MacDonald type [2+2]
     condensation is described.  In this method a bisformyl dipyrrylmethane is
     treated with a biscarboxydipyrrylmethane.  Attempts to obtain the
     .delta.-meso-monoaryl protoporphyrin [I; R1R2 = H, R3 = Ph (IV)] by the
     a,c-biladiene method failed as it could not be prepd. starting from its
     tripyrrene precursor (V).  The synthesis of the V is described.  Mol.
     modeling studies allowed us to find the most favorable conformations for
     II and III.  In both porphyrins, the exocyclic Ph group adopts a
     noncoplanar disposition relative to the plane of the macrocycle.  In
     porphyrin III the macrocycle is nearly planar while nonplanar saddle
     conformation was obtained for porphyrin II.
IT     ***309757-24-2P***
     RL: PNU (Preparation, unclassified); PREP (Preparation)
        (attempted prepn. of)
RN   309757-24-2  CAPLUS
CN   21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethenyl-3,7,12,17-
     tetramethyl-5-phenyl-, dimethyl ester (9CI)  (CA INDEX NAME)


/ Structure 1 in file .gra /

RE.CNT  23     THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7   ANSWER 2 OF 11  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1999:367089  CAPLUS
DN   131:110291
TI   A convenient synthesis of a Ru(bpy)3-based catenane-type triad and its
     incorporation into a protein scaffold
AU   Hu, Yi-Zhen; Tsukiji, Shinya; Shinkai, Seiji; Hamachi, Itaru
CS   Department of Chemistry and Biochemistry, Graduate School of Engineering,
     Kyushu University, Fukuoka, 812-8581, Japan
SO   Chemistry Letters (1999), (6), 517-518
     CODEN: CMLTAG; ISSN: 0366-7022
PB   Chemical Society of Japan
DT   Journal
LA   English
AB   A catenated heme cofactor consisting of a sensitizer (Ru(bpy)2L (L = I)),
     a donor (protoheme) II (R = 4'-methyl-2,2'-bipyridin-4-yl) and an accepto
```

(cyclobis(paraquat-p-phenylene) (III)) was prepd. by stepwise coordination, followed by Fe-insertion. Reconstitution of apomyoglobin with this cofactor afforded a protein-based, noncovalently-linked photosynthetic triad.

IT ***231302-74-2P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reactant for prepn. of iron porphyrinate ruthenium bipyridine bipryidinocrown ether catenated with cyclobisparaquatphenylene for incorporation in protein scaffold)

RN 231302-74-2 CAPLUS

CN Ruthenium(1+), (2,5,8,11,14,27,30,33,36,39-decaoxa-19,22-diazatetracyclo[38.2.2.116,20.121,25]hexatetraconta-16,18,20(46),21,23,25(45),40,42,43-nonaene-.kappa.N19,.kappa.N22)[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-[[2-[3-(4'-methyl[2,2'-bipyridin]-4yl-.kappa.N1,.kappa.N1')propoxy]ethyl]amino]-3-oxopropyl]-21H,23H-porphin 2-propanoato(1-)](4,4'-dimethyl-2,2'-bipyridine-.kappa.N1,.kappa.N1')-, (OC-6-43)-, chloride, monohydrochloride, catena compd. with 5,12,19,26-tetraazoniaheptacyclo[24.2.2.22,5.27,10.212,15.216,19.221,24]t traconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene tetrachloride (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 235438-51-4
CMF C96 H110 N11 O14 Ru . Cl H . Cl
CCI CCS

/ Structure 2 in file .gra /

/ Structure 3 in file .gra /

/ Structure 4 in file .gra /

CM 2

CRN 117271-78-0
CMF C36 H32 N4 . 4 Cl

/ Structure 5 in file .gra /

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 11 CAPLUS

AN 1997:528290 CAPLUS
DN 127:109178

TI Molecular Modeling of a Functionalized Aib-Based Octapeptide by Molecular Mechanics Calculations Restrained by NMR and Fluorescence Data in DMSO

AU Pispisa, B.; Palleschi, A.; Amato, M. E.; Segre, A. L.; Venanzi, M.
CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor Vergata, Rome, 00133, Italy

SO Macromolecules (1997), 30(17), 4905-4910
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal

LA English
AB The structural features of the sequential octapeptide Boc-(Leu)2-Lys(P)-(Aib)2-(Leu)2-Lys(N)-OCMe3, where P is protoporphyrin IX and N is naphthalene, were investigated in DMSO by NMR and fluorescence spectroscopy. Earlier IR, CD, and fluorescence results showed that this compd. attains a 310-helical conformation in methanol or water/methanol (75/25, vol./vol.). By contrast, the backbone structure in DMSO is destroyed, but the high helix propensity of the Aib residues forces the peptide to attain locally ordered arrangements, reminiscent of .beta.-tur features. Both NMR coupling const. and NOE connectivity data allowed the computation of the structural features of part of the mol., but only thei combination with fluorescence results allowed the construction of the whole mol. model. Implications of fluorescence data on the dynamics of internal rotation of the chromophores are briefly discussed.
IT ***171736-16-6***
RL: PRP (Properties)
(conformation of aminoisobutyric acid peptide by by mol. mechanics calcns. restrained by NMR and fluorescence data in DMSO)
RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2 carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 6 in file .gra /

/ Structure 7 in file .gra /

/ Structure 8 in file .gra /

L7 ANSWER 4 OF 11 CAPLUS
AN 1996:641877 CAPLUS
DN 125:328358
TI Synthesis, stereochemical and photophysical studies of chiral mesoporphyrins
AU Poignant, Geraldine; Bourseul, Annie; Geze, Catherine; Plouzennec, Maryvonne Le; Le Maux, Paul; Bondon, Arnaud; Simonneaux, Gerard; Moinet, Claude; Vonarx, Veronique; Patrice, Thierry
CS Lab. Chim. Organometallique Biol., CNRS, Rennes, 35042, Fr.
SO Tetrahedron Letters (1996), 37(42), 7511-7514
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB The synthesis and NMR characterization of chiral mesoporphyrins bearing .alpha.-methoxy-.alpha.-(trifluoromethyl)phenylacetyl residues are reported. The phototoxicity with circular polarized light and intracellular localization in L1210 cells are also described as preliminary results.
IT ***183558-97-6P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biologica study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, stereochem. and photophys. studies of chiral mesoporphyrins)
RN 183558-97-6 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethyl-3,7,12,17-tetramethy
5-[(3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl)amino]-, dimethyl
ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 9 in file .gra /

L7 ANSWER 5 OF 11 CAPLUS
AN 1996:189170 CAPLUS
DN 124:317836
TI Conformational Statistics and Energetics Analysis of Sequential Peptides
Undergoing Intramolecular Transfer of Excitation Energy
AU Pispisa, B.; Palleschi, A.; Venanzi, M.; Zanotti, G.
CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor
Vergata, Rome, 00133, Italy
SO Journal of Physical Chemistry (1996), 100(16), 6835-44
CODEN: JPCHAX; ISSN: 0022-3654
PB American Chemical Society
DT Journal
LA English
AB The photophysics of short linear peptides of general formula
Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OCMe3 [AA = Ala, n = 1-4; AA =
.alpha.-aminoisobutyric acid (Aib), n = 1-2; P = protoporphyrin IX, N =
1-naphthylacetyl] were investigated in 75/25 (vol./vol.) water/methanol b
steady-state and time-resolved fluorescence expts. Quenching of the
excited naphthyl chromophore takes place by electronic energy transfer to
the porphyrin ground state, and proceeds on a time scale of 3-8 ns. A
minor and slower fluorescence lifetime measures the decay of the
exciplexes. Quenching efficiencies exhibit a different trend, depending
on whether AA = Ala or Aib, indicating differences in the structural
features of the two series of peptides. Consistently, CD spectra suggest
that the former compds. populate .alpha.-helical structures, while the
latter ones possibly attain a 310-helix conformation, in agreement with
the proven ability of Aib to form 310-helixes in soln. The increased
percentage of intramol. H-bonds in the P(Aib)nN as compared to the
corresponding P(Ala)nN peptides, as detd. by IR spectra in dil. CD3OD or
CDCl3 soln., confirms this conclusion. The fluorescence results were
satisfactorily described by a dipole-dipole interaction mechanism,
provided the mutual orientations of N and P groups are taken into account
which implies that interconversion among conformational substrates of
chromophore linkage is slow on the time scale of the transfer process.
Conformational statistics anal. shows a rather wide interprobe sepn.
distance distribution for each peptide, owing to the aliph. portion of th
side-chains carrying the chromophores, but theor. conformational anal.
indicates that only a few energetically favored conformers are the major
contributors to the energy transfer process.
IT ***171736-14-4*** ***171736-16-6***
RL: PRP (Properties)
(conformational statistics and energetics anal. of sequential peptides
undergoing intramol. transfer of excitation energy)
RN 171736-14-4 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,1
tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-
dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-
leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 10 in file .gra /

/ Structure 11 in file .gra /

/ Structure 12 in file .gra /

RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2 carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 13 in file .gra /

/ Structure 14 in file .gra /

/ Structure 15 in file .gra /

L7 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:819429 CAPLUS
DN 124:30371
TI Intramolecular electronic energy transfer in peptides carrying naphthalen and protoporphyrin molecules: a spectroscopy and conformational statistic investigation
AU Pispisa, B.; Venanzi, M.; Palleschi, A.; Zanotti, G.
CS Dip. Science, Univ. Rome, Rome, 00133, Italy
SO Biopolymers (1995), 36(4), 497-510
CODEN: BIPMAA; ISSN: 0006-3525
PB Wiley
DT Journal
LA English
AB Short linear peptides, carrying an AA spacer in the backbone chain (AA = Aib or Ala) and naphthalene (N) and protoporphyrin IX (P) covalently boun to .epsilon.-amino groups of lysine side chains, were synthesized. The general formula is Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OtBu (n = 0-2) The photophys. behavior of these compds. was investigated in water/methanol (75/25, vol./vol.) soln. by steady-state and time-resolved fluorescence expts. Quenching of excited naphthyl chromophore takes plac by electronic energy transfer to the porphyrin ground state and proceeds on a time scale of 3-8 ns, while a minor and slower (.apprxeq.45 ns) fluorescence lifetime measures the decay of the exciplexes. The results were compared with those obtained earlier for the P(Ala)nN peptides (n = 0-4) in methanol soln., showing that addn. of water does not significantl alter the dynamic relaxation behavior of the systems investigated, but affects the dissipation mechanism of the energy transferred to P. Quenching efficiencies from both fluorescence intensity and fluorescence lifetime measurement follow a different trend as the no. of AA units increases, depending on whether AA = Aib or Ala, indicating that there ar differences in the structural features of the two series of peptides. Consistently, CD spectral results suggest that the former compds. attain ordered conformations, possibly of the 310-helical type, while the latter populate .alpha.-helical structures to an extent depending on the chain length. Their IR data in dil. CD3OD or CDCl3 soln. confirm this conclusion in that there is an increased percentage of intramol. H bonds

in the P(Aib)nN as compared to the corresponding P(Ala)nN peptides. The photophys. results can be well described by a long-range dipole-dipole interaction model, provided the sepn. distances distribution and mutual orientation of N and P groups are taken into account. The need for using the angular relationships between the probes implies that interconversion among conformational substrates of chromophore linkages is slow on the time scale of the transfer process, very likely because of both the amide bond in the linkages and the bulkiness of the donor-acceptor pair.

IT ***171736-17-7*** ***171736-18-8*** ***171736-19-9***
RL: PRP (Properties)
(intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)

RN 171736-17-7 CAPLUS

CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,1 tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-leucyl] L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 16 in file .gra /

/ Structure 17 in file .gra /

/ Structure 18 in file .gra /

RN 171736-18-8 CAPLUS

CN L-Lysine, N2-[N-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-alanyl] L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 19 in file .gra /

/ Structure 20 in file .gra /

/ Structure 21 in file .gra /

RN 171736-19-9 CAPLUS

CN L-Lysine, N2-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-leucyl]-L-leucyl] N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 22 in file .gra /

/ Structure 23 in file .gra /

IT ***171736-14-4P*** ***171736-16-6P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)
RN 171736-14-4 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,1 tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 24 in file .gra /

/ Structure 25 in file .gra /

/ Structure 26 in file .gra /

RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2 carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 27 in file .gra /

/ Structure 28 in file .gra /

/ Structure 29 in file .gra /

L7 ANSWER 7 OF 11 CAPLUS
AN 1988:21587 CAPLUS
DN 108:21587
TI Synthetic and biosynthetic studies of porphyrins. Part 11. The synthesi of meso oxygenated protoporphyrins
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (2), 307-12
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 108:21587
AB Protoporphyrin IX di-Me ester (I; R-R3 = H) was treated with (BzO)2 to give a mixt. of 4 meso-benzoyloxy derivs. I (R = OBz, R1-R3 = H; R1 = OBz R = R2 = R3 = H; R2 = OBz, R = R1 = R3 = H; R3 = OBz, R-R2 = H) (II). Th mixt. II was hydrolyzed to the corresponding oxyporphyrins, complexed wit Fe, and oxidized with mol. O to give 4 biliverdin di-Me esters III.

Conditions for the HPLC sepns. of II and III are discussed.
IT ***83807-58-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and basic hydrolysis of)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 30 in file .gra /

L7 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:202979 CAPLUS
DN 104:202979
TI On the mechanism of the chemical and enzymic oxygenations of .alpha.-oxyprotohemin IX to iron.cntdot.biliverdin IX.alpha.
AU Sano, Seiyo; Sano, Toyo; Morishima, Isao; Shiro, Yoshitugu; Maeda, Yutaka
CS Dep. Public Health, Fac. Med., Kyoto, 606, Japan
SO Proceedings of the National Academy of Sciences of the United States of America (1986), 83(3), 531-5
CODEN: PNASA6; ISSN: 0027-8424
DT Journal
LA English
AB .alpha.-Oxyprotohemin IX (I), an early intermediate in heme catabolism, was synthesized and its autoxidn. to biliverdin IX.alpha. was studied. I anaerobic aq. pyridine, I (hexacoordinated) underwent autoredn. to yield an Fe(II)-I .pi.-neutral radical bis(pyridine) complex, which reacted wit an equimolar amt. of O2 to give verdohemochrome IX.alpha. (II)-pyridine and CO in 75-80% yield via an intermediate with an absorption max. at 893 nm. II did not react with further O2. Reconstituted apomyoglobin-I complex (pentacoordinated) reacted with an equimolar amt. of O2 to form a Fe(II)-oxyporphyrin .pi.-neutral radical intermediate, which rearranged t a green compd. (.lambda.max 660 and 704 nm) with elision of CO. The gree product, which is probably an apomyoglobin-verdoheme .pi.-radical complex reacted with another equimolar amt. of O2 to give Fe(III)-biliverdin IX.alpha.. Demetallation of this gave biliverdin IX.alpha. in an overall yield of 70-75%. Apparently, the 2-step sequence of oxyheme autoxidn. in the presence of apomyoglobin is .alpha.-oxyprotoheme IX .fwdarw. II .pi.-radical .fwdarw. Fe(III)-biliverdin IX.alpha. (with CO leaving in th 1st step). A similar mechanism may prevail in vivo.the hexa- and pentacoordinated Fe(II) .pi.-radical form of the oxyporphyrin is crucial in triggering the autoxidn. of the complex to verdohemochrome IX.alpha.. The hexa- and pentacoordinated Fe(II) .pi.-radical form of the oxyporphyrin was crucial in triggering the autoxidn. of the complex to II Further oxygenation of II to Fe(III)-biliverdin IX.alpha. occurred only i the pentacoordinated apomyoglobin-verdoheme Fe(II) complex.
IT ***83807-58-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of and iron insertion in)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 31 in file .gra /

L7 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:45748 CAPLUS
DN 98:45748
TI Heminopeptide complexes which are models of an "active center" of

oxygen-transferring hemoproteides. Synthesis and properties
AU Kazakova, N. A.; Radyukhin, V. A.; Luzgina, V. N.; Filippovich, E. I.; Kamyshan, N. V.; Kudryavtseva, E. V.; Evstigneeva, R. P.
CS Mosk. Inst. Tonkoi Khim. Tekhnol., Moscow, USSR
SO Zhurnal Obshchei Khimii (1982), 52(8), 1896-906
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
AB Unsym. 6(7), 7(6)-bis(amino acyl)peptide derivs. of protohemin IX (models of active centers of Hb and myoglobin) were prepd. The stability consts. were detd. for the mono- and bis(amino acyl)peptide derivs. of protohemin IX with axial N-contg. ligands (1-methylimidazole); the covalently-bound peptide has a stabilizing effect on the formation and stability of the 5-coordinate complexes. The hydrophobic spatial environment around the F ion of the ferroporphyrin 5-coordinate complexes affects their stability toward oxidn. and their ability to coordinate CO at room temp.
IT ***83841-59-2D*** , iron complexes with methylimidazole and pyridine
RL: PRP (Properties)
(stability consts. of)
RN 83841-59-2 CAPLUS
CN L-Cysteine, N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethy 21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl-L-leucyl-L-alanyl-L-phenylalanyl-L-alanyl-S-(phenylmethyl)-, 6-methyl ester, (1.fwdarw.1')-amide with L-leucyl-1-(phenylmethyl)-L-histidyl-N6-[(phenylmethoxy)carbonyl]-L-lysine methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 32 in file .gra /

/ Structure 33 in file .gra /

L7 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:615860 CAPLUS
DN 97:215860
TI Synthesis of the four meso-oxyprotoporphyrin isomers
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Chemical Communications (1982), (14), 794-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB Oxidn. of protoporphyrin IX di-Me ester with Bz2O2 in PhCl at 95.degree. for 5 min gave a mixt. of the 4 title compds. I (1 of R-R3 = OBz, other R groups = H) in 20% yield. I were sepd. by h.p.l.c. and identified by conversion to the corresponding biliverdins by passage in a 1:1 CHCl3/C6H soln. through a column of basic Al2O3, conversion to Fe complexes, and oxygenation in pyridine.
IT ***83807-58-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to corresponding biliverdin)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 34 in file .gra /

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L7   ANSWER 11 OF 11  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1980:621062  CAPLUS
DN   93:221062
TI   Unsymmetrical 6,7-peptidylprotohemin IX
IN   Molokoedov, A. S.; Radyukhin, V. A.; Filippovich, E. I.; Evstigneeva, R.
     P.
PA   Moscow Institute of Fine Chemical Technology, USSR
SO   U.S.S.R.
     From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1980, (7), 117.
     CODEN: URXXAF
DT   Patent
LA   Russian
FAN.CNT 1
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
PI   SU 717039          T    19800225      SU 1978-2606603  19780331
                                           SU 1978-2606603  19780331
AB   Title compds. I [R = PhCH2O, Leu-His(CH2Ph)-Lys(Z)-OMe (Z = PhCH2O2C), R1
     = Leu-His-Ala-Lys(Z)-Gly-Cys(CH2Ph)-OCH2Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH2Ph
     OCH2Ph; R = Leu-His-Ala-Lys(Z)-Gly-Cys(CH2Ph)-OCH2Ph, Ala-Leu-Ala-Phe-Ala
     Cys(CH2Ph)-OCH2Ph, R1 = PhCH2O, Leu-His(CH2Ph)-Lys(Z)-OMe] were prepd. by
     esterifying I (R = PhCH2O, R1 = HO; R = HO, R1 = PhCH2O) with C6H5OH by
     the mixed anhydride method with ClCO2Et and condensing the resulting
     pentachlorophenyl active esters with the appropriate hexapeptides in 2.5-
     M urea soln. at 40-45.degree..
IT     ***75561-35-2DP***  , complex with iron chloride
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN   75561-35-2  CAPLUS
CN   L-Cysteine, N-[N-[N-[N-[N-[N-[3-[8,13-diethenyl-3,7,12,17-tetramethyl-18-
     [3-oxo-3-(phenylmethoxy)propyl]-21H,23H-porphin-2-yl]-1-oxopropyl]-L-
     alanyl]-L-leucyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]-S-(phenylmethyl)-,
     phenylmethyl ester (9CI)  (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 35 in file .gra /



/ Structure 36 in file .gra /



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=>
Uploading C:\STNEXP4\QUERIES\867d.str

L9      STRUCTURE UPLOADED

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                                                        ENTRY   SESSION
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DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> s l8
SAMPLE SEARCH INITIATED 14:57:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     21 TO ITERATE

100.0% PROCESSED      21 ITERATIONS                           0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          146 TO      694
PROJECTED ANSWERS:               0 TO        0

L10            0 SEA SSS SAM L8

=> search l8
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:58:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    363 TO ITERATE

100.0% PROCESSED     363 ITERATIONS                           0 ANSWERS
SEARCH TIME: 00.00.01

L11            0 SEA SSS FUL L8

=> s l9
SAMPLE SEARCH INITIATED 14:58:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     22 TO ITERATE

100.0% PROCESSED      22 ITERATIONS                           0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          159 TO      721
PROJECTED ANSWERS:               0 TO        0

L12            0 SEA SSS SAM L9
```

```
=> search l9
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:58:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    421 TO ITERATE

100.0% PROCESSED     421 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L13           0 SEA SSS FUL L9

=>
Uploading C:\STNEXP4\QUERIES\867e.str

L14      STRUCTURE UPLOADED

=> s l14
SAMPLE SEARCH INITIATED 15:00:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      22 TO ITERATE

100.0% PROCESSED      22 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          159 TO      721
PROJECTED ANSWERS:               0 TO        0

L15           0 SEA SSS SAM L14

=> search l14
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:00:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    421 TO ITERATE

100.0% PROCESSED     421 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L16           0 SEA SSS FUL L14

=>
Uploading C:\STNEXP4\QUERIES\867f.str

L17      STRUCTURE UPLOADED

=> s l17
SAMPLE SEARCH INITIATED 15:01:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      21 TO ITERATE

100.0% PROCESSED      21 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          146 TO      694
PROJECTED ANSWERS:               0 TO        0

L18           0 SEA SSS SAM L17

=> search l17
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
```

```
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:01:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    363 TO ITERATE

100.0% PROCESSED     363 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

L19           2 SEA SSS FUL L17

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   623.36    1002.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -7.62

FILE 'CAPLUS' ENTERED AT 15:02:53 ON 03 MAY 2004
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FILE COVERS 1907 - 3 May 2004  VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004  (20040502/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l19
L20           1 L19

=> d l19 fbib ab hitstr
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n


=> d l20 fbib ab hitstr

L20  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1982:607121  CAPLUS
DN   97:207121
TI   Synthesis of mono-S-aminoacyl derivatives of cobalt-porphyrin complexes
     containing peptides
AU   Kazakova, N. A.; Nguyen Huy Doan; Filippovich, E. I.; Evstigneeva, R. P.
CS   USSR
SO   Deposited Doc. (1980), SPSTL 287khp-D80, 13 pp.  Avail.: SPSTL
DT   Report
LA   Russian
AB   I (R = CH2:CH, H, COMe; R1 = R2 = OH) were converted to I (R = CH2:CH, H,
     COMe; R1 = LeuHisOMe, LeuHisAlaLysGlyCys(CH2Ph)OCH2Ph,
     LeuHisAlaPheAlaGlyOMe, R2 = OH or vice versa).  The peptide-contg. Co
```

porphyrins were characterized by IR spectra and electronic spectra. Thes complexes are easily oxidized in air and are reduced by Na2S2O6 as indicated by electronic spectral data.

IT ***83118-03-0P*** ***83139-86-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 83118-03-0 CAPLUS

CN Cobaltate(1-), [1-methyl-N-[N-[N-[N-[N-[N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-leucyl]-L-histidyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]glycinato(3-)-N21,N22,N23,N24]-, hydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)

/ Structure 37 in file .gra /

/ Structure 38 in file .gra /

RN 83139-86-0 CAPLUS

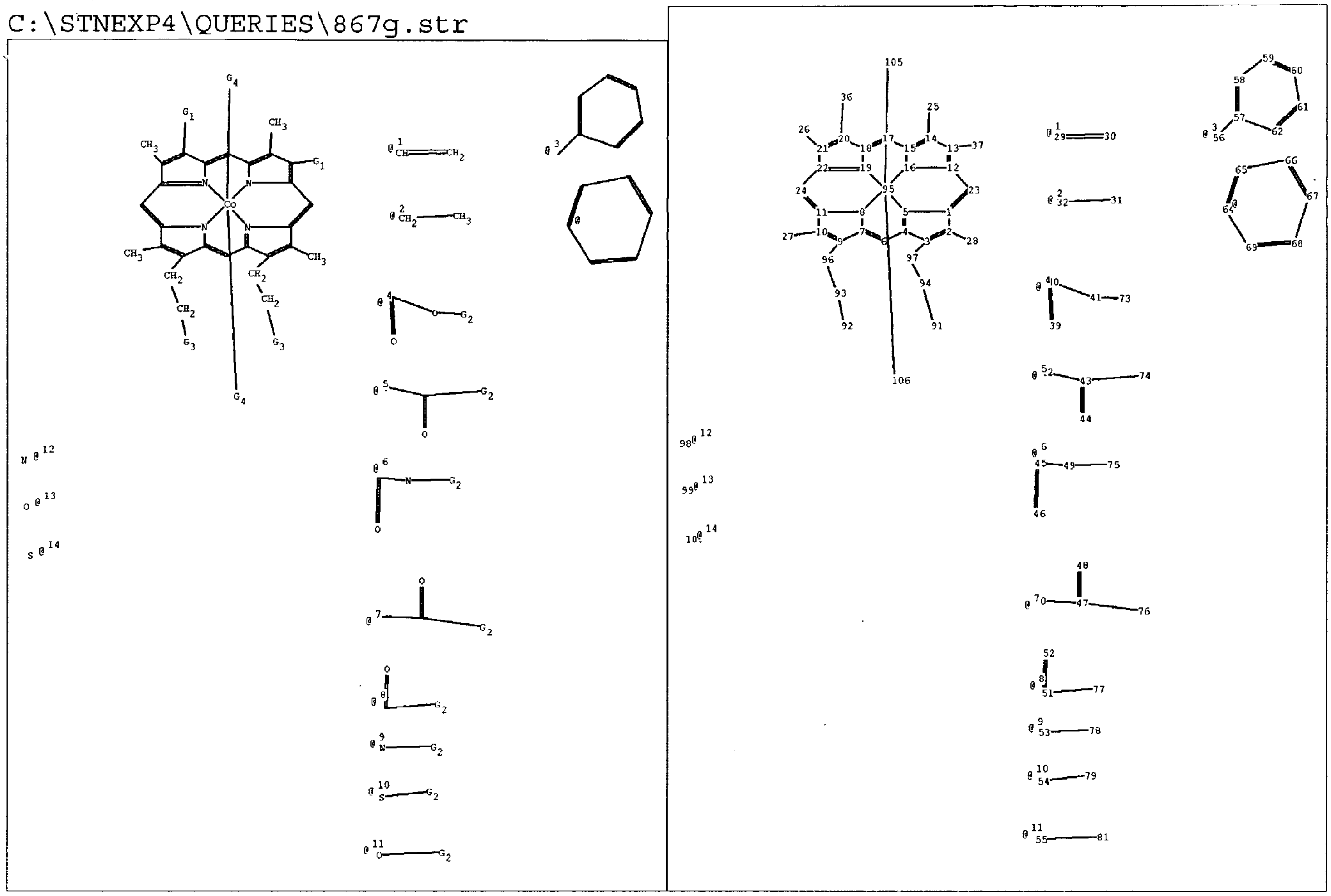
CN Cobaltate(1-), [1-(phenylmethyl) N-[N-[N2-[N-[N-[N-[3-[18-(2-carboxyethyl 8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L leucyl]-L-histidyl]-L-alanyl]-N6-[(phenylmethoxy)carbonyl]-L-lysyl]glycyl S-(phenylmethyl)-L-cysteinato(3-)-N21,N22,N23,N24]-, hydrogen, (SP-4-2)-(9CI) (CA INDEX NAME)

/ Structure 39 in file .gra /

/ Structure 40 in file .gra /

=>

C:\STNEXP4\QUERIES\867g.str



chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 96 97 105 106

ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 95

ring/chain nodes :
98 99 100

chain bonds :
2-28 3-97 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-96 94-97 95-105 95-106

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-95 6-7 7-8 7-9 8-11 8-95
9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
16-95 17-18 18-19 18-20 19-22 19-95 20-21 21-22 22-24 57-58
57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
68-69

exact/norm bonds :
5-95 7-8 8-11 8-95 12-16 13-37 15-16 16-95 19-95 20-36 39-40
40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
49-75 51-52 51-77 53-78 54-79 55-81 91-94 92-93 95-105 95-106

exact bonds :
2-28 3-97 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-96
94-97

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

G1:[*1],[*2]

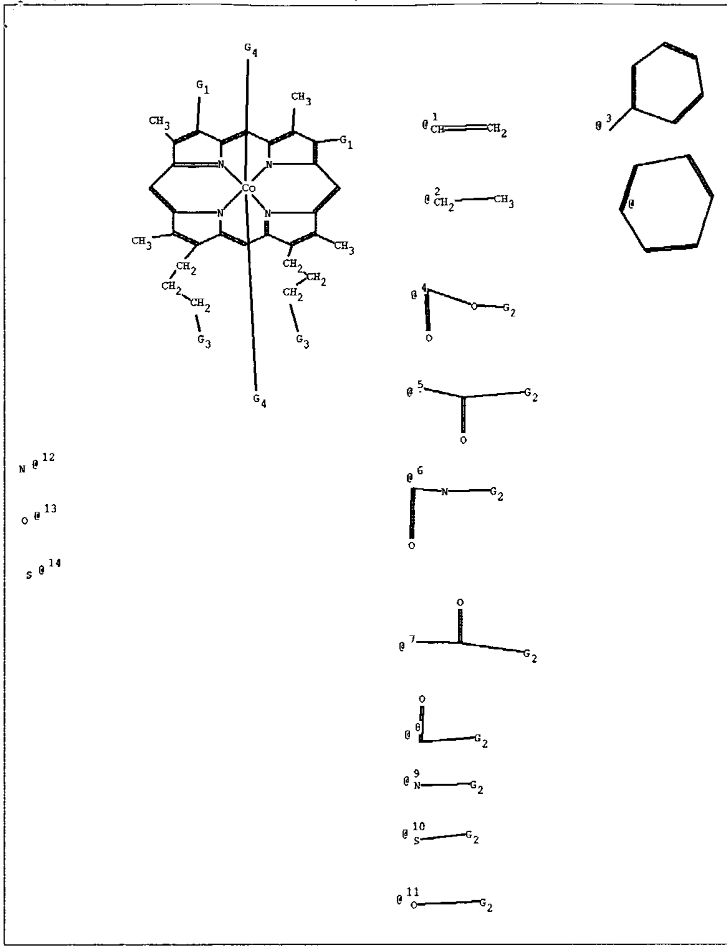
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

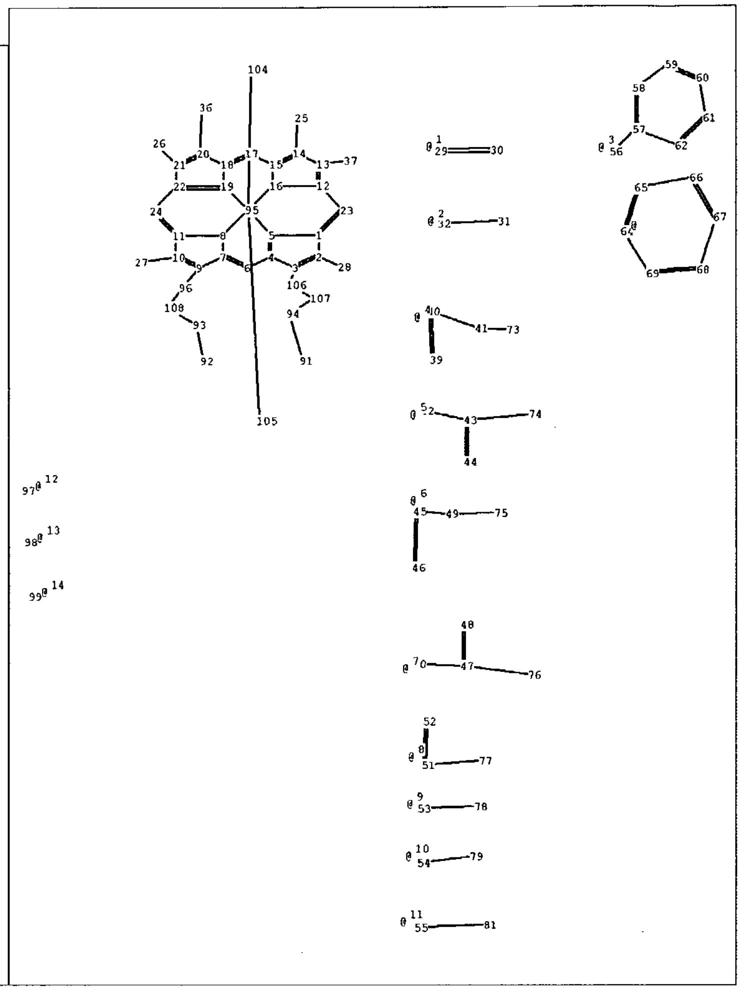
G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

G4:X,[*12],[*13],[*14]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:CLASS 79:CLASS 81:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS
95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS 100:CLASS 105:CLASS
106:CLASS

C:\STNEXP4\QUERIES\867h.str





chain nodes :
25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 96 104 105 106 107 108
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 95
ring/chain nodes :
97 98 99
chain bonds :
2-28 3-106 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-108 94-107 95-104 95-105 96-108 106-107
ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-95 6-7 7-8 7-9 8-11 8-95
9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
16-95 17-18 18-19 18-20 19-22 19-95 20-21 21-22 22-24 57-58
57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
68-69
exact/norm bonds :
5-95 7-8 8-11 8-95 12-16 13-37 15-16 16-95 19-95 20-36 39-40
40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
49-75 51-52 51-77 53-78 54-79 55-81 91-94 92-93 95-104 95-105
exact bonds :
2-28 3-106 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-108
94-107 96-108 106-107
normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

G4:X,[*12],[*13],[*14]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:CLASS 79:CLASS 81:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS
95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS 104:CLASS 105:CLASS
106:CLASS 107:CLASS 108:CLASS

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptau129pxo

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 15:06:15 ON 03 MAY 2004
FILE 'CAPLUS' ENTERED AT 15:06:15 ON 03 MAY 2004

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.63	1007.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-8.31

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.63	1007.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-8.31

FILE 'REGISTRY' ENTERED AT 15:06:26 ON 03 MAY 2004
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\867h.str

L21   STRUCTURE UPLOADED

```
=>
Uploading C:\STNEXP4\QUERIES\867g.str

L22      STRUCTURE UPLOADED

=> s l21
SAMPLE SEARCH INITIATED 15:11:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      13 TO ITERATE

100.0% PROCESSED      13 ITERATIONS                            0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:            44 TO       476
PROJECTED ANSWERS:                0 TO         0

L23            0 SEA SSS SAM L21

=> search l21
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:11:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    265 TO ITERATE

100.0% PROCESSED     265 ITERATIONS                            0 ANSWERS
SEARCH TIME: 00.00.01

L24            0 SEA SSS FUL L21

=> s l22
SAMPLE SEARCH INITIATED 15:11:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      14 TO ITERATE

100.0% PROCESSED      14 ITERATIONS                            0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:            56 TO       504
PROJECTED ANSWERS:                0 TO         0

L25            0 SEA SSS SAM L22

=> search l22
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:11:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    241 TO ITERATE

100.0% PROCESSED     241 ITERATIONS                            0 ANSWERS
SEARCH TIME: 00.00.01

L26            0 SEA SSS FUL L22
```